Metal/Catalyst-Free Sequential C-N Bond Forming Cascades at Room Temperature: Environment-Friendly One-Pot Synthesis of 5-Aminoimidazoles from Aryl Glyoxals, Anilines and Amidines

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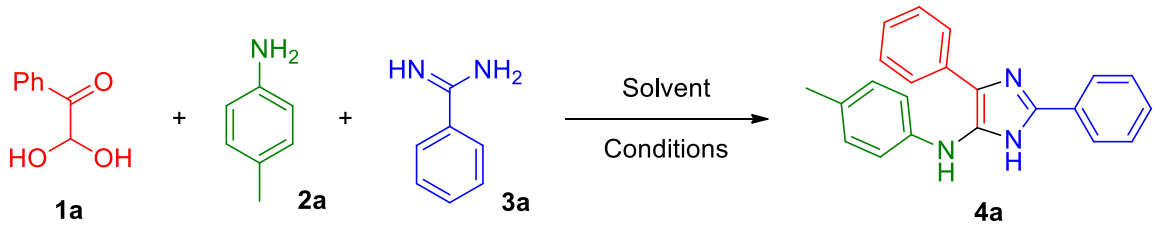
Supporting Information

Table of Contents

Table 1. Optimization of the Reaction Conditions[a]

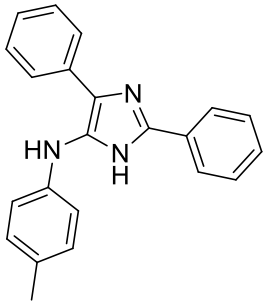


Entry	Stoichiometry	Condition	Yield %
1	**1a** + **2a** (1.0 equiv.) in EtOH, stir for 1 h; then **3a**-HCl (1.1 equiv.) + TEA (1.5 equiv.)	55 ℃, 6 h	56
2	**1a** + **2a** (1.0 equiv.) in EtOH, stir for 1 h; then **3a**-HCl (1.1 equiv.) +K_2CO_3 (1.5 equiv.)	55 ℃, 6 h	58
3	**1a** + **2a** (1.0 equiv.) in EtOH, stir for 2 h; then **3a**-free base (1.1 equiv.)	55 ℃, 6 h	60
4	**1a** (1.0 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	62
5	**1a** (1.1 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	73
6	**1a** (1.2 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	86
7	**1a** (1.3 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	83
8	**1a** (1.2 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (1.8 equiv.)	RT, 16 h	68
9	**1a** (1.2 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.2 equiv.)	RT, 16 h	86
10	**1a** (1.3 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	55 ℃, 16 h	69
11	**1a** (1.3 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h 50 ℃; then **3a** (2.0 equiv.)	55 ℃, 16 h	49
12	**1a** (1.2 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then AcOH (0.2 equiv.) **3a** (2 equiv.)	RT, 16 h	50
13	**1a** (1.2 equiv.) in MeOH, + **2a** (1.0 equiv.) stir for 3 h; then *p*-TSA (0.2 equiv.) **3a** (2.0 equiv.)	RT, 16 h	73
14	**1a** (1.2 equiv.) in EtOH, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	68
15	**1a** (1.2 equiv.) in IPA, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	55
16	**1a** (1.2 equiv.) in THF, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	18
17	**1a** (1.2 equiv.) in DMF, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	07
18	**1a** (1.2 equiv.) in DMSO, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	13
19	**1a** (1.2 equiv.) in ACN, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	22
20	**1a** (1.2 equiv.) in DCM, + **2a** (1.0 equiv.) stir for 3 h; then **3a** (2.0 equiv.)	RT, 16 h	20

[a] All reactions were performed with **2a** (1.0 mmol).

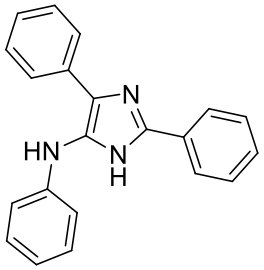
General procedure one-pot synthesis of highly substituted imidazoles (4a-4aq). Aniline (1.0 mmol) was added to a stirred solution of glyoxal (1.2 mmol) in MeOH (5 mL) and stirred for 1.5 h at rt. To this mixture, benzaimidine (2.0 mmol) was added and stirred for additional 16 h. The reaction mass was concentrated under reduced pressure and the residue was purified by silica gel column chromatography (EtOAc in *n*-hexane).

2,4-Diphenyl-*N*-(*p*-tolyl)-1*H*-imidazol-5-amine (4a).



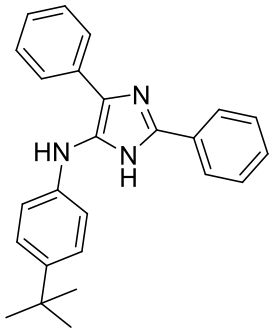
Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4a** as white solid (0.28 g, yield 88%), mp 145−147 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.93 (d, J = 7.6 Hz, 2H), 7.73 (d, J = 7.2 Hz, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.37 (d, J = 7.2 Hz, 1H), 7.31 (t, J = 7.6 Hz, 2H), 7.19 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 8.0 Hz, 2H), 6.63 (d, J = 8.0 Hz, 2H), 2.18 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 145.89, 145.34, 131.39, 130.51, 129.82, 129.69, 129.49, 128.23, 127.66, 126.96, 126.60, 114.93, 20.55. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{20}N_3$ 326.1657; found 326.1648.

***N*,2,5-Triphenyl-1*H*-imidazol-5-amine.**



Purification by silica gel column chromatography (0 to 13% EtOAc in *n*-hexane) afforded **4b** as light yellow solid (0.22 g, yield 71%), mp 158−160 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 8.8 Hz, 2H), 7.74 (d, J = 8.4 Hz, 2H), 7.45 (t, J = 8.4 Hz, 2H), 7.39 (t, J = 7.6 Hz, 1H), 7.32 (t, J = 7.6 Hz, 2H), 7.20 (t, J = 7.6 Hz, 1H), 7.10 (t, J = 8.8 Hz, 2H), 6.72 (d, J = 8.0 Hz, 2H), 6.67 (t, J = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ 148.35, 145.47, 131.36, 130.03, 129.82, 129.73, 129.51, 127.75, 126.98, 126.62, 119.11, 114.82. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{18}N_3$ 312.1501; found 312.1489.

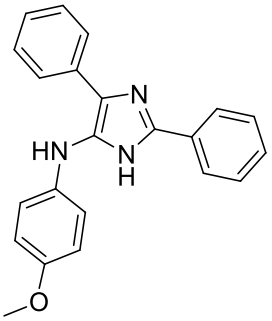
_N_-(4-(Tert-butyl)phenyl)-2,4-diphenyl-1_H_-imidazol-5-amine (4c).



Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4c** as white solid (0.32 g, yield 86%), mp 208−209 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 7.2 Hz, 2H), 7.45 (t, J = 7.6 Hz, 2H), 7.38 (d, J = 7.2 Hz, 1H), 7.33 (t, J = 7.2 Hz, 2H), 7.21 (d, J = 7.6 Hz, 1H), 7.16 (d, J = 7.6 Hz, 2H), 6.67 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 145.88, 145.38, 141.93, 131.47,

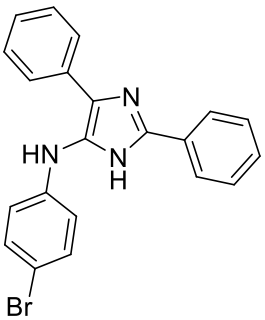
129.88, 129.75, 129.56, 127.72, 127.02, 126.83, 126.66, 114.65, 34.74, 32.06. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{25}H_{26}N_3$ 368.2127; found 368.2118.

_N_-(4-Methoxyphenyl)-2,5-diphenyl-1_H_-imidazol-5-amine (4d).



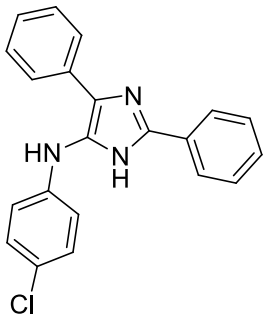
Purification by silica gel column chromatography (0 to 17% EtOAc in *n*-hexane) afforded **4d** as brown solid (0.24 g, yield 71%), mp 175−177 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 8.8 Hz, 2H), 7.74 (d, J = 7.2 Hz, 2H), 7.45 (t, J = 7.2 Hz, 2H), 7.38 (d, J = 7.6 Hz, 1H), 7.32 (t, J = 8.0 Hz, 2H), 7.20 (t, J = 7.6 Hz, 1H), 6.74 (d, J = 8.8 Hz, 2H), 6.69 (d, J = 8.8 Hz, 2H), 3.69 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 153.97, 145.28, 142.11, 131.38, 129.81, 129.66, 129.49, 127.61, 126.92, 126.58, 116.00, 115.72, 56.12 . HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{20}N_3O$ 342.1606; found 342.1595.

_N_-(4-Bromophenyl)-2,5-diphenyl-1_H_-imidazol-5-amine (4e).



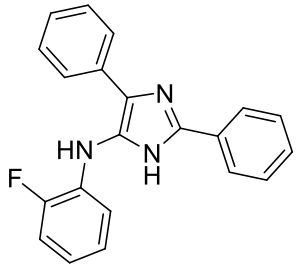
Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded 4e as off-white solid (0.37 g, yield 95%), mp 138−140 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 7.6 Hz, 2H), 7.71 (d, J = 7.6 Hz, 2H), 7.45 (t, J = 8.0 Hz, 2H), 7.39 (d, J = 7.2 Hz, 1H), 7.36 (t, J = 8.0 Hz, 2H), 7.23 (t, J = 7.6 Hz, 1H), 7.20 (d, J = 7.2 Hz, 2H), 6.66 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.59, 145.63, 132.75, 131.23, 129.82, 129.79, 129.58, 127.91, 126.96, 126.62, 116.50, 110.46. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{17}N_3Br$ 390.0606; found 390.0598.

_N_-(4-Chlorophenyl)-2,5-diphenyl-1_H_-imidazol-5-amine (4f).



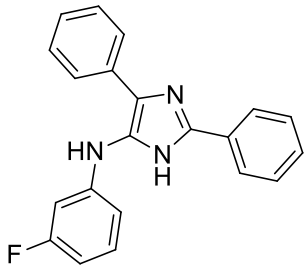
Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4f** as off-white solid (0.33 g, yield 94%), mp 145−147 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 7.6 Hz, 2H), 7.72 (d, J = 7.2 Hz, 2H), 7.45 (t, J = 7.6 Hz, 2H), 7.39 (d, J = 7.2 Hz, 1H), 7.36 (t, J = 7.6 Hz, 2H), 7.22 (t, J = 7.2 Hz, 1H), 7.07 (d, J = 8.0 Hz, 2H), 6.70 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.17, 145.62, 131.26, 129.83, 129.58, 127.90, 126.97, 126.63, 123.50, 116.01. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{17}N_3Cl$ 346.1111; found 346.1100.

_N_-(2-Fluorophenyl)-2,5-diphenyl-1_H_-imidazol-5-amine (4g).



Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4g** as white solid (0.32 g, yield 96%), mp 184−186 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.95 (d, J = 7.6 Hz, 2H), 7.74 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.39 (d, J = 7.6 Hz, 1H), 7.34 (t, J = 8.0 Hz, 2H), 7.22 (t, J = 7.2 Hz, 1H), 7.03 (dd, J = 12.4, 8.0 Hz, 1H), 6.85 (t, J = 8.0 Hz, 1H), 6.67 (d, J = 8.0 Hz, 1H), 6.63 (d, J = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ 154.15, 151.78, 145.86, 136.35, 136.24, 131.29, 129.88, 129.62, 129.31, 128.03, 126.97, 126.67, 125.45, 119.09, 115.79, 115.61; ^{19}F NMR (376 MHz, CD_3OD): δ -137.82. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{17}N_3F$ 330.1407; found 330.1397.

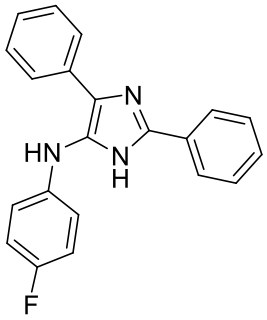
***N*-(3-Fluorophenyl)-2,5-diphenyl-1*H*-imidazol-5-amine (4h).**



Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4h** as white solid (0.32 g, yield 98%), mp 187−189 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.95 (d, J = 7.2 Hz, 2H), 7.72 (d, J = 7.2 Hz, 2H), 7.46 (d, J = 8.0 Hz, 2H), 7.40 (d, J = 7.6 Hz, 1H), 7.35 (t, J = 7.2 Hz, 2H), 7.23 (t, J = 7.2 Hz, 1H), 7.08 (q, J = 7.6 Hz, 1H),

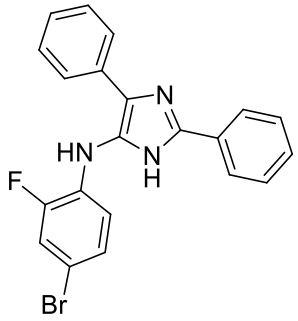
6.53 (d, *J* = 7.6 Hz, 1H), 6.42 (d, *J* = 12.0 Hz, 1H), 6.36 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ 166.62, 164.22, 150.60, 150.50, 145.70, 131.35, 131.27, 129.85, 129.60, 127.97, 127.01, 126.66, 110.63, 105.27, 105.04, 101.48, 101.23; ^{19}F NMR (376 MHz, CD_3OD): δ -115.38. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{17}N_3F$ 330.1407; found 330.1405.

_N_-(4-Fluorophenyl)-2,4-diphenyl-1_H_-imidazol-5-amine (4i).



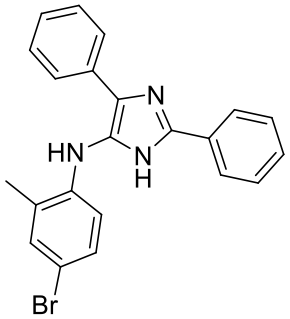
Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4i** as white solid (0.32 g, yield 97%), mp 150−152 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, *J* = 7.6 Hz, 2H), 7.73 (d, *J* = 7.2 Hz, 2H), 7.45 (t, *J* = 7.6 Hz, 2H), 7.38 (d, *J* = 7.2 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.21 (t, *J* = 7.2 Hz, 1H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.68−6.71 (m, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 158.70, 156.37, 145.51, 144.70, 131.34, 129.84, 129.77, 129.55, 127.81, 126.96, 126.63, 116.38, 116.15, 115.74, 115.66; ^{19}F NMR (376 MHz, CD_3OD): δ -129.81. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{17}N_3F$ 330.1407; found 330.1397.

_N_-(4-Bromo-2-fluorophenyl)-2,5-diphenyl-1_H_-imidazol-5-amine (4j).



Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4j** as white solid (0.33 g, yield 81%), mp 180−182 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 7.6 Hz, 2H), 7.72 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.2 Hz, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.36 (t, J = 7.6 Hz, 2H), 7.24 (t, J = 8.0 Hz, 2H), 7.00 (d, J = 8.4 Hz, 1H), 6.58 (t, J = 9.6 Hz, 1H); ^{13}C NMR (100 MHz, CD_3O): δ 153.85, 151.42, 145.94, 136.03, 135.91, 131.25, 129.98, 129.93, 129.73, 128.49, 128.22, 127.04, 126.72, 119.27, 119.05, 116.86, 108.99; ^{19}F NMR (376 MHz, CD_3OD): δ -134.34 (triplets). HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3FBr$ 408.0512; found 408.0503.

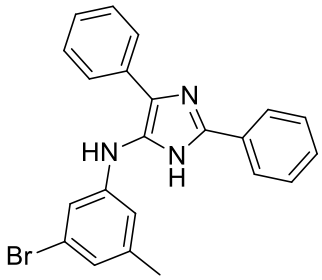
***N*-(2-Fluorophenyl)-2,5-diphenyl-1*H*-imidazol-5-amine (4k).**



Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4k** as white solid (0.38 g, yield 93%), mp 147−149 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 8.0 Hz, 2H), 7.69 (d, J = 7.2 Hz, 2H), 7.45 (t, J = 7.6 Hz, 2H), 7.39 (d, J = 7.2 Hz, 1H), 7.33 (t, J = 8.0 Hz, 2H), 7.22 (d, J = 7.2 Hz, 1H), 7.20 (s, 1H), 7.01 (d, J =

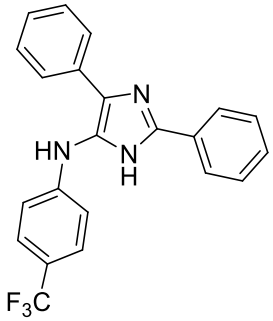
8.8 Hz, 1H), 6.41 (d, *J* = 8.8 Hz, 1H); ^{13}C {^{1}H} NMR (100 MHz, CD_3OD): δ 145.75, 145.61, 133.66, 131.28, 130.33, 129.89, 129.86, 129.60, 127.94, 126.90, 126.63, 126.22, 115.24, 110.67, 17.77. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_3Br$ 404.0762; found 404.0753.

_N_-(3-Bromo-5-methylphenyl)-2,5-diphenyl-1_H_-imidazol-5-amine (4l).



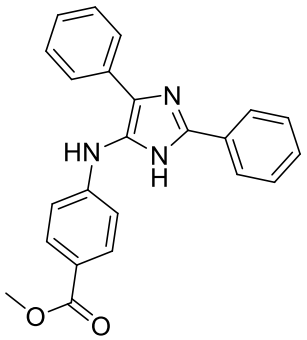
Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4k** as white solid (0.39 g, yield 97%), mp 218−220 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.95 (d, *J* = 7.6 Hz, 2H), 7.71 (d, *J* = 7.2 Hz, 2H), 7.46 (t, *J* = 7.2 Hz, 2H), 7.40 (d, *J* = 7.2 Hz, 1H), 7.36 (t, *J* = 8.0 Hz, 2H), 7.23 (t, *J* = 7.2 Hz, 1H), 6.68 (s,1H), 6.64 (s, 1H), 6.60 (s, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ 149.84, 145.72, 141.93, 131.28, 129.86, 129.85, 129.62, 127.99, 127.03, 126.68, 123.78, 122.47, 114.73, 114.15, 21.39. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_3Br$ 404.0762; found 404.0755.

2,5-Diphenyl-_N_-[4-(trifluoromethyl)phenyl]-1_H_-imidazol-5-amine (4m).



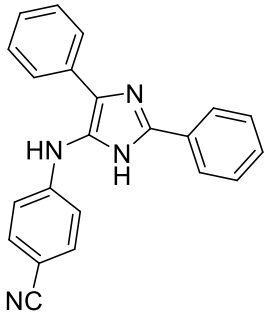
Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4m** as white solid (0.35 g, yield 91%), mp 208−210 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.95 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.40−7.33 (m, 5H), 7.24 (t, J = 7.6 Hz, 1H), 6.82 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 151.70, 145.85, 131.23, 129.93, 129.90, 129.68, 128.13, 127.84, 127.40, 127.36, 127.05, 126.69, 125.16, 114.21; ^{19}F NMR (376 MHz, CD_3OD): δ -62.55. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{17}N_3F_3$ 380.1375; found 380.1356.

Methyl 4-[(2,5-diphenyl-1*H*-imidazol-5-yl)amino]benzoate (4n).



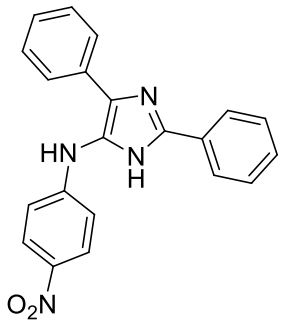
Purification by silica gel column chromatography (0 to 25% EtOAc in *n*-hexane) afforded **4n** as white solid (0.35 g, yield 95%), mp 140−142 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.95 (d, J = 7.6 Hz, 2H), 7.79 (d, J = 8.8 Hz, 2H), 7.70 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.2 Hz, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.35 (t, J = 7.2 Hz, 2H), 7.23 (t, J = 7.2 Hz, 1H), 6.76 (d, J = 7.2 Hz, 2H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 169.12, 153.21, 145.96, 132.42, 131.25, 129.99, 129.95, 129.72, 128.21, 127.12, 126.74, 119.99, 113.90, 52.08. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{20}N_3O_2$ 370.1556; found 370.1545.

4-[(2,5-Diphenyl-1*H*-imidazol-5-yl)amino]benzonitrile (4o).



Purification by silica gel column chromatography (0 to 25% EtOAc in *n*-hexane) afforded **4o** as white solid (0.23 g, yield 69%), mp 129−131 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.95 (d, J = 7.6 Hz, 2H), 7.68 (d, J = 7.6 Hz, 2H), 7.48 (t, J = 7.2 Hz, 2H), 7.44 (d, J = 7.6 Hz, 2H), 7.39 (d, J = 7.2 Hz, 1H), 7.36 (t, J = 8.0 Hz, 2H), 7.25 (t, J = 7.2 Hz, 1H), 6.68 (d, J = 7.2 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 152.76, 146.12, 134.69, 131.19, 130.06, 129.96, 129.78, 128.35, 127.14, 126.75, 121.23, 114.83, 100.26. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{17}N_4$ 337.1453; found 337.1442.

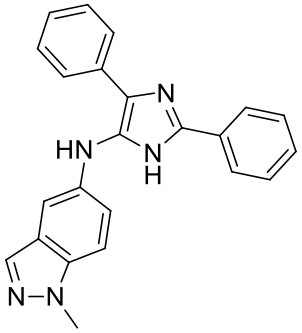
_N_-(4-Nitrophenyl)-2,5-diphenyl-1_H_-imidazol-5-amine (4p).



Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4p** as white solid (0.15 g, yield 41%), mp 217−219 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 8.04 (d, J = 8.8 Hz, 2H), 7.96 (d, J = 7.6 Hz, 2H), 7.68 (t, J = 7.6 Hz, 2H), 7.46 (t, J = 7.2 Hz, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.36 (t, J = 7.6 Hz, 2H), 7.25 (t, J = 7.6 Hz, 1H), 6.91 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 154.68, 146.19, 139.86, 131.07,

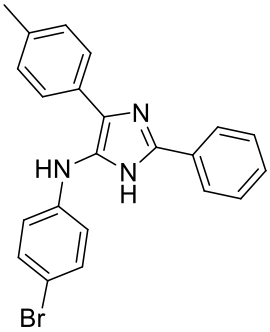
130.07, 129.92, 129.78, 128.42, 127.15, 126.99, 126.73, 113.74. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{17}N_4O_2$ 357.1352; found 357.1348.

_N_-(2,5-Diphenyl-1_H_-imidazol-5-yl)-1-methyl-1_H_-indazol-5-amine (4q).



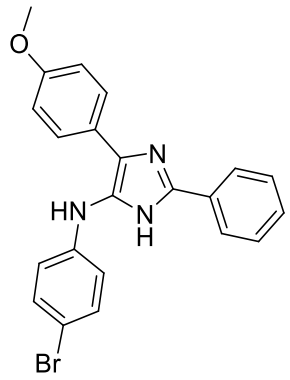
Purification by silica gel column chromatography (0 to 35% EtOAc in *n*-hexane) afforded **4p** as white solid (0.20 g, yield 55%), mp 114−116 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (s, 1H), 7.92 (s, 1H), 7.73 (d, J = 8.4 Hz, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.36 (t, J = 8.4 Hz, 1H), 7.32 (t, J = 8.4 Hz, 2H), 7.19 (t, J = 7.6 Hz, 1H), 6.73 (d, J = 8.8 Hz, 2H), 6.68 (d, J = 8.8 Hz, 2H), 3.68 (s,3H); ^{13}C NMR (100 MHz, CD_3OD): δ 145.52, 142.92, 136.94, 132.30, 131.39, 129.95, 129.78, 128.68, 127.75, 126.89, 126.57, 126.98, 119.55, 110.94, 102.36, 35.35 . HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{23}H_{20}N_5$ 366.1719; found 366.1707.

_N_-(4-Bromophenyl)-2-phenyl-5-(_p_-tolyl)-1_H_-imidazol-5-amine (4r).



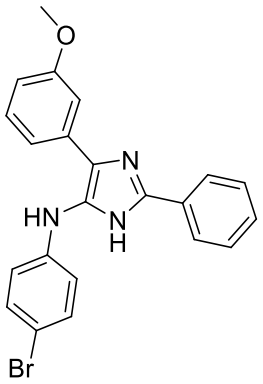
Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4r** as white solid (0.37 g, yield 92%), mp 109−111 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.92 (d, J = 7.6 Hz, 2H), 7.69 (d, J = 7.6 Hz, 2H), 7.42 (t, J = 7.2 Hz, 2H), 7.35 (t, J = 7.2 Hz, 1H), 7.18 (d, J = 7.6 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 6.63 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.72, 145.35, 137.89, 132.74, 131.29, 130.22, 130.12, 129.82, 129.72, 126.92, 126.57, 11.46, 110.34, 21.24. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_3Br$ 404.0762; found 404.0755.

***N*-(4-Bromophenyl)-5-(4-methoxyphenyl)-2-phenyl-1*H*-imidazol-5-amine (4s).**



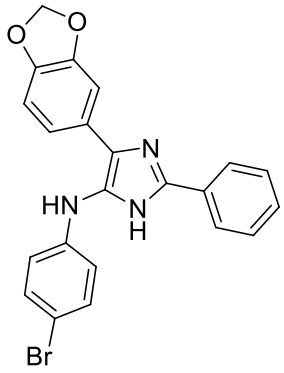
Purification by silica gel column chromatography (0 to 13% EtOAc in *n*-hexane) afforded **4s** as off white solid (0.31 g, yield 75%), mp 190−192 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.92 (d, J = 8.4 Hz, 2H), 7.63 (d, J = 7.6 Hz, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.56 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 8.4 Hz, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.37 (t, J = 7.6 Hz, 1H), 7.19 (d, J = 8.4 Hz, 2H), 6.91 (d, J = 8.4 Hz, 2H), 6.63 (d, J = 8.4 Hz, 2H), 3.78 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 160.23, 147.88, 145.11, 132.75, 131.34, 129.83, 129.66, 128.40, 126.51, 116.41, 115.03, 114.30, 110.30, 55.68. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_3OBr$ 420.0712; found 420.0698.

***N*-(4-Bromophenyl)-5-(3-methoxyphenyl)-2-phenyl-1*H*-imidazol-5-amine (4t).**



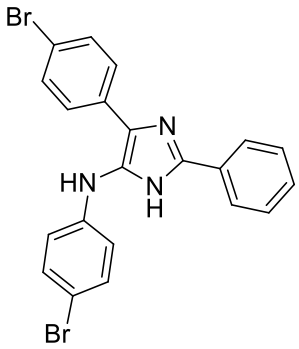
Purification by silica gel column chromatography (0 to 15% EtOAc in *n*-hexane) afforded **4t** as white solid (0.27 g, yield 66%), mp 101−103 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 7.6 Hz, 2H), 7.44 (t, J = 7.6 Hz, 2H), 7.37 (t, J = 7.2 Hz, 1H), 7.31 (d, J = 7.6 Hz, 1H), 7.30 (s, 1H), 7.25 (t, J = 8.4 Hz, 1H), 7.20 (d, J = 8.8 Hz, 2H), 6.77 (d, J = 8.4 Hz, 1H), 6.65 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 161.26, 147.60, 145.62, 132.80, 131.23, 130.60, 129.85, 126.67, 119.22, 116.50, 1113.99, 112.09, 110.47, 55.52. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_3OBr$ 420.0712; found 420.0692.

5-(Benzo[d][1,3]dioxol-5-yl)-*N*-(4-bromophenyl)-2-phenyl-1*H*-imidazol-5-amine (4u).



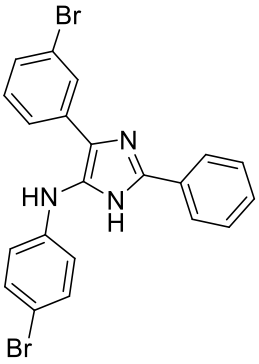
Purification by silica gel column chromatography (0 to 25% EtOAc in *n*-hexane) afforded **4u** as white solid (0.30 g, yield 69%), mp 117−119 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.91 (d, J = 7.2 Hz, 2H), 7.44 (t, J = 7.4 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.24−7.19 (m, 4H), 6.82 (d, J = 8.4 Hz, 1H), 6.63 (d, J = 8.4 Hz, 2H), 5.93 (s, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 149.33, 148.11, 147.73, 145.20, 142.02, 132.79, 131.29, 129.85, 129.75, 129.01, 126.56, 126.22, 120.87, 116.44, 110.47, 109.36, 107.58, 102.42. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{17}N_3O_2Br$ 434.0504; found 434.0498.

_N_,5-Bis(4-bromophenyl)-2-phenyl-1_H_-imidazol-5-amine (4v).



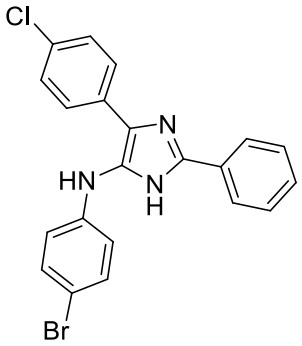
Purification by silica gel column chromatography (0 to 14% EtOAc in *n*-hexane) afforded **4v** as off white solid (0.30 g, yield 64%), mp 176−178 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.93 (d, J = 7.6 Hz, 2H), 7.65 (d, J = 8.4 Hz, 2H), 7.49 (d, J = 8.4 Hz, 2H), 7.43 (t, J = 8.0 Hz, 2H), 7.39 (t, J = 8.0 Hz, 1H), 7.22 (d, J = 8.4 Hz, 2H), 6.65 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.27, 145.98, 132.85, 132.66, 131.11, 129.95, 129.86, 128.55, 126.65, 121.42, 116.55, 110.73. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3Br_2$ 467.9711; found 467.9702.

5-(3-Bromophenyl)-_N_-(4-bromophenyl)-2-phenyl-1_H_-imidazol-5-amine (4w).



Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4w** as off white solid (0.32 g, yield 69%), mp 96−98 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.95 (s, 1H), 7.94 (d, *J* = 8.0 Hz, 2H), 7.71 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 8.0 Hz, 2H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.36 (d, *J* = 7.0 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.8 Hz, 2H), 6.66 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.22, 146.28, 132.87, 131.30, 131.10, 130.56, 130.01, 129.88, 129.59, 129.56, 126.71, 125.48, 123.66, 116.61, 110.78. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3Br_2$ 467.9711; found 467.9703.

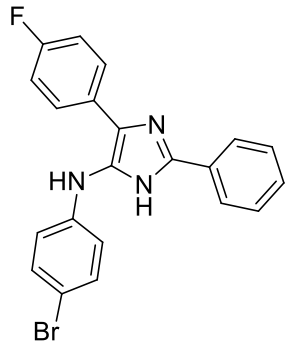
***N*-(4-Bromophenyl)-5-(4-chlorophenyl)-2-phenyl-1*H*-imidazol-5-amine (4x).**



Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4x** as white solid (0.40 g, yield 94%), mp 162−164 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.71 (t, *J* = 8.0 Hz, 2H), 7.45 (t, *J* = 7.2 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 1H), 7.31 (d, *J* = 8.8 Hz, 2H), 7.21 (d, *J* = 8.8 Hz, 2H), 6.65 (d, *J* = 8.8 Hz, 2H);

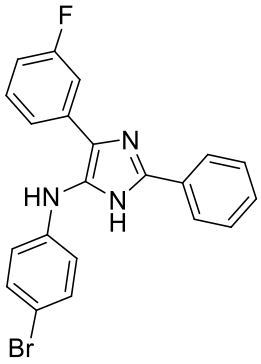
^{13}C NMR (100 MHz, CD_3OD): δ 147.35, 145.97, 133.48, 132.86, 131.14, 129.95, 129.87,129.68, 128.31, 126.66, 116.56, 110.71. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3ClBr$ 424.0216; found 424.0208.

_N_-(4-Bromophenyl)-5-(4-fluorophenyl)-2-phenyl-1_H_-imidazol-5-amine (4y).



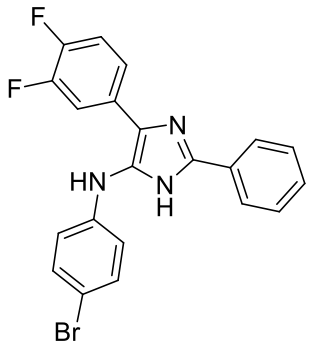
Purification by silica gel column chromatography (0 to 15% EtOAc in *n*-hexane) afforded **4y** as white solid (0.40 g, yield 97%), mp 123−125 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.93 (d, J = 7.6 Hz, 2H), 7.73 (t, J = 6.0 Hz, 2H), 7.45 (t, J = 7.2 Hz, 2H), 7.38 (t, J = 7.2 Hz, 1H), 7.21 (d, J = 8.8 Hz, 2H), 7.08 (t, J = 8.8 Hz, 2H), 6.64 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 164.43, 161.99, 147.66, 145.72, 132.87, 131.27, 130.30, 129.91, 129.04, 128.96, 126.65, 116.51, 116.39, 116.28, 110.58; ^{19}F NMR (376 MHz, CD_3OD): δ -126.85. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3BrF$ 408.0512; found 408.0502.

_N_-(4-Bromophenyl)-5-(3-fluorophenyl)-2-phenyl-1_H_-imidazol-5-amine (4z).



Purification by silica gel column chromatography (0 to 12% EtOAc in *n*-hexane) afforded **4z** as off white solid (0.22 g, yield 55%), mp 106−108 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (d, J = 7.6 Hz, 2H), 7.56 (d, J = 7.6 Hz, 1H), 7.51 (d, J = 10.8 Hz, 1H), 7.45 (t, J = 7.2 Hz, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.31 (q, J = 7.6 Hz, 1H), 7.22 (d, J = 8.4 Hz, 2H), 6.94 (t, J = 8.0 Hz, 1H), 6.66 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 165.65, 163.23, 147.29, 132.87, 131.38, 131.30, 131.11, 130.02, 129.89, 126.72, 122.60, 116.56, 114.42, 114.21, 113.49, 113.26, 110.76; ^{19}F NMR (376 MHz, CD_3OD): δ -114.84. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3Br$ F 408.0512; found 408.0499.

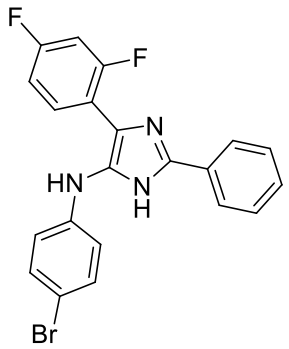
N-(4-Bromophenyl)-5-(3,4-difluorophenyl)-2-phenyl-1*H*-imidazol-5-amine (4aa).



Purification by silica gel column chromatography (0 to 15% EtOAc in *n*-hexane) afforded **4aa** as white solid (0.41 g, yield 96%), mp 182−184 °C. ^{1}H NMR (400 MHz,

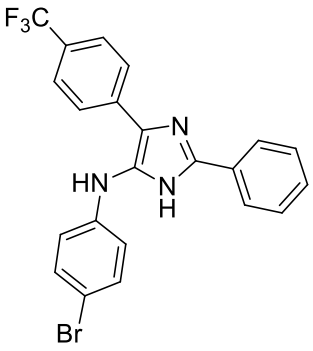
CD_3OD): δ 7.93 (d, J = 7.6 Hz, 2H), 7.65 (t, J = 9.6 Hz, 1H), 7.53 (brs, 1H), 7.45 (t, J = 7.6 Hz, 2H), 7.39 (t, J = 7.6 Hz, 1H), 7.26−7.20 (m, 3H), 6.65 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 152.83, 152.70, 151.57, 151.44, 150.38, 150.25, 149.11, 148.98, 147.16, 146.01, 132.91, 131.05, 130.00, 129.87, 126.65, 123.38, 123.34, 123.28, 118.50, 118.32, 116.54, 115.75, 115.56, 110.92; ^{19}F NMR (376 MHz, CD_3OD): δ -140.18, -142.51. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{15}N_3BrF_2$ 426.0417; found 426.0406.

_N_-(4-Bromophenyl)-5-(2,4-difluorophenyl)-2-phenyl-1_H_-imidazol-5-amine (4ab).



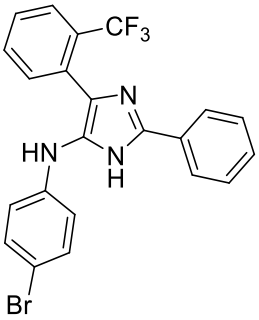
Purification by silica gel column chromatography (0 to 15% EtOAc in *n*-hexane) afforded **4ab** as white solid (0.31 g, yield 73%), mp 166−168 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.90 (d, J = 8.0 Hz, 2H), 7.56 (q, J = 8.4 Hz, 1H), 7.44 (t, J = 7.2 Hz, 2H), 7.37 (t, J = 7.2 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H), 7.03 (brs, 1H), 6.97 (t, J = 7.6 Hz, 1H), 6.69 (d, J = 6.0 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 163.73, 163.62, 161.26, 161.14, 145.99, 144.55, 131.25, 131.06, 129.75, 128.48, 125.10, 115.19, 111.22, 111.03, 109.14, 103.93, 103.67, 103.61; ^{19}F NMR (376 MHz, CD_3OD): δ -111.40, -112.20. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{15}N_3F_2Br$ 426.0417; found 426.0410.

_N_-(4-Bromophenyl)-2-phenyl-5-(4-(trifluoromethyl)phenyl)-1_H_-imidazol-5-amine (4ac).



Purification by silica gel column chromatography (0 to 15% EtOAc in *n*-hexane) afforded **4ac** as white solid (0.43 g, yield 93%), mp 124−126 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.94 (t, J = 7.6 Hz, 4H), 7.64 (d, J = 7.6 Hz, 2H), 7.47 (t, J = 7.2 Hz, 2H), 7.40 (t, J = 7.2 Hz, 1H), 7.24 (d, J = 7.6 Hz, 2H), 6.70 (d, J = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.06, 146.54, 132.93, 131.06, 130.14, 129.91, 129.39, 129.07, 127.10, 126.98, 126.78, 126.48, 126.44, 124.40, 116.69, 110.97; ^{19}F NMR (376 MHz, CD_3OD): δ -63.99. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{16}N_3F_3Br$ 458.0480; found 458.0471.

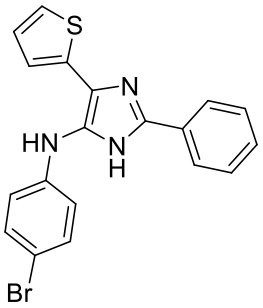
***N*-(4-Bromophenyl)-2-phenyl-5-(2-(trifluoromethyl)phenyl)-1*H*-imidazol-5-amine (4ad).**



Purification by silica gel column chromatography (0 to 25% EtOAc in *n*-hexane) afforded **4ad** as white solid (0.17 g, yield 37%), mp 208−210 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.87 (d, J = 8.4 Hz, 2H), 7.79 (d, J = 8.4 Hz, 1H), 7.62 (d, J = 8.8 Hz, 1H), 7.56 (d, J = 8.4 Hz, 1H), 7.54 (d, J = 8.4 Hz, 1H), 7.44 (t, J = 7.6 Hz, 2H), 7.37 (t, J = 7.6 Hz, 1H), 7.16 (d, J = 8.4 Hz, 2H), 6.69 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.78,

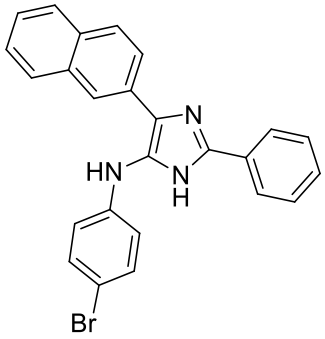
145.25, 134.53, 132.97, 132.53, 131.27, 131.22, 130.92, 129.98, 129.91, 129.80, 127.48, 127.42, 127.37, 127.32, 126.83, 126.39, 124.12, 116.64, 110.38; ^{19}F NMR (376 MHz, CD_3OD): δ -60.53. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{16}N_3F_3Br$ 458.0480; found 458.0467.

_N_-(4-Bromophenyl)-2-phenyl-5-(thiophen-2-yl)-1_H_-imidazol-5-amine (4ae).



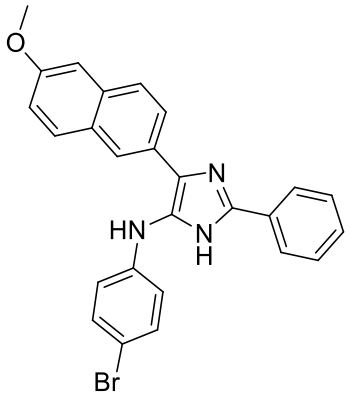
Purification by silica gel column chromatography (0 to 17% EtOAc in *n*-hexane) afforded **4ae** as white solid (0.26 g, yield 67%), mp 140−143 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.93 (d, *J* = 7.6 Hz, 2H), 7.45 (t, *J* = 7.2 Hz, 2H), 7.39 (d, *J* = 7.2 Hz, 1H), 7.38 (d, *J* = 7.2 Hz, 1H), 7.29 (d, *J* = 4.8 Hz, 1H), 7.21 (d, *J* = 8.8 Hz, 2H), 7.02 (t, *J* = 4.8 Hz, 1H), 6.64 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.48, 145.61, 132.80, 131.15, 129.96, 129.92, 129.75, 129.68, 127.98, 126.66, 125.63, 124.16, 116.55, 110.64. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{19}H_{15}N_3SBr$ 396.0170; found 396.0164.

_N_-(4-Bromophenyl)-5-(naphthalen-2-yl)-2-phenyl-1_H_-imidazol-5-amine (4af).



Purification by silica gel column chromatography (0 to 10% EtOAc in *n*-hexane) afforded **4af** as off white solid (0.25 g, yield 58%), mp 180−183 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 8.18 (brs, 1H), 7.98 (d, *J* = 7.2 Hz, 2H), 7.89 (d, *J* = 7.6 Hz, 1H), 7.80 (t, *J* = 7.6 Hz, 3H), 7.50−7.36 (m, 5H), 7.22 (d, *J* = 8.8 Hz, 2H), 6.72 (t, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.69, 135.03, 133.80, 132.87, 131.31, 129.94, 129.24, 129.20, 129.03, 128.66, 127.41, 126.94, 126.74, 125.32, 125.23, 116.68. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{25}H_{19}N_3Br$ 440.0762; found 440.0747.

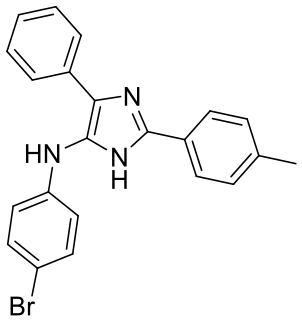
_N_-(4-Bromophenyl)-5-(6-methoxynaphthalen-2-yl)-2-phenyl-1_H_-imidazol-5-amine (4ag).



Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4ag** as off white solid (0.37 g, yield 80 %), mp 207−209 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 8.09 (s, 1H), 7.97 (d, *J* = 8.0 Hz, 2H), 7.83 (d, *J* = 8.0 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.46 (t, *J* = 8.8 Hz, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.21 (t, *J*

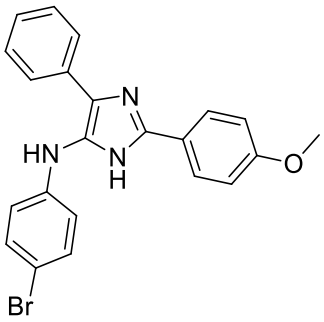
= 8.8 Hz, 2H), 7.19 (s, 1H), 7.11 (d, *J* = 8.8 Hz, 1H), 6.70 (d, *J* = 8.4 Hz, 2H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 161.80, 150.29, 148.14, 137.53, 135.31, 133.83, 132.97, 132.87, 132.39, 132.31, 130.62, 129.14, 128.22, 127.78, 122..65, 119.09, 112.95, 109.20, 58.25HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{26}H_{21}N_3OBr$ 470.0868; found 470.0866.

_N_-(4-Bromophenyl)-5-phenyl-2-(_p_-tolyl)-1_H_-imidazol-5-amine (4ah).



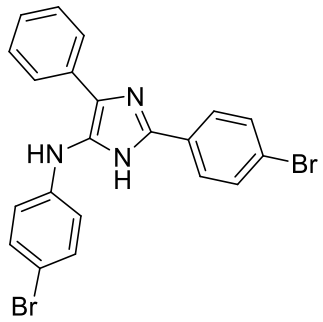
Purification by silica gel column chromatography (0 to 13% EtOAc in *n*-hexane) afforded **4ah** as off white solid (0.38 g, yield 94%), mp 188−190 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.82 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.65 (d, *J* = 8.4 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.72, 145.89, 140.09, 132.77, 131.73, 130.47, 129.59, 128.53, 127.87, 126.93, 126.67, 126.65, 116.48, 110.40, 21.33. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_3Br$ 404.0762; found 404.0747.

_N_-(4-Bromophenyl)-2-(4-methoxyphenyl)-5-phenyl-1_H_-imidazol-5-amine (4ai).



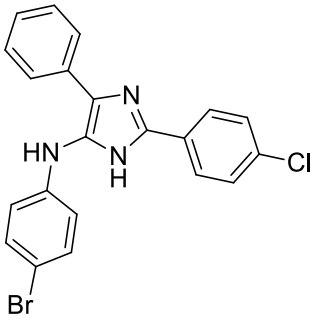
Purification by silica gel column chromatography (0 to 25% EtOAc in *n*-hexane) afforded **4ai** as white solid (0.38 g, yield 90%), mp 215−217 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.87 (d, J = 8.8 Hz, 2H), 7.70 (d, J = 7.2 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.22 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 7.2 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 6.65 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 161.80, 147.78, 145.90, 132.76, 129.59, 128.19, 127.78, 126.84, 123.98, 116.47, 115.22, 110.34, 55.81. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{19}N_3OBr$ 420.0712; found 420.0699.

***N*,2-Bis(4-bromophenyl)-5-phenyl-1*H*-imidazol-5-amine (4aj).**



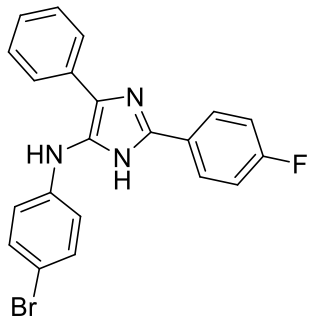
Purification by silica gel column chromatography (0 to 11% EtOAc in *n*-hexane) afforded **4aj** as white solid (0.37 g, yield 80%), mp 213−215 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.84 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 7.2 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 7.6 Hz, 2H), 6.66 (d, J = 7.6 Hz, 2H); ^{13}CNMR (100 MHz, CD_3OD): δ 147.48, 144.42,132.99, 132.77, 130.32, 129.62, 128.25, 128.05, 126.99, 123.66, 116.53, 110.54. HRMS (ESI) *m/z* calcd for $C_{21}H_{16}N_3Br_2$, $[M + H]^+$ 467.9711; found: 467.9702.

N-(4-Bromophenyl)-2-(4-chlorophenyl)-5-phenyl-1*H*-imidazol-5-amine (4ak).



Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4ak** as white solid (0.36 g, yield 83%), mp 205−207 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.92 (d, J = 8.4 Hz, 2H), 7.71 (d, J = 7.2 Hz, 2H), 7.46 (d, J = 8.4 Hz, 2H), 7.35 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 7.6 Hz, 2H), 6.66 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.55, 144.42, 135.60, 132.78, 130.01, 129.64, 128.06, 127.00, 116.52, 110.53. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3ClBr$ 424.0216; found 424.0199.

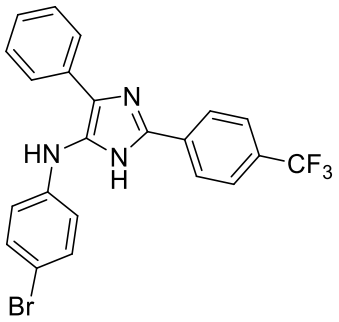
_N_-(4-Bromophenyl)-2-(4-fluorophenyl)-5-phenyl-1_H_-imidazol-5-amine (4al).



Purification by silica gel column chromatography (0 to 13% EtOAc in *n*-hexane) afforded **4al** as white solid (0.37 g, yield 90%), mp 174−175 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 7.96 (dd, J = 8.8, 5.6 Hz, 2H), 7.71 (d, J = 8.0 Hz, 2H), 7.35 (t, J = 8.0 Hz, 2H), 7.25−7.17 (m, 5H), 6.66 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 165.70, 163.24, 147.63, 144.76, 132.78, 129.62, 128.82, 128.73, 127.98, 127.78, 126.94, 116.82, 116.60,

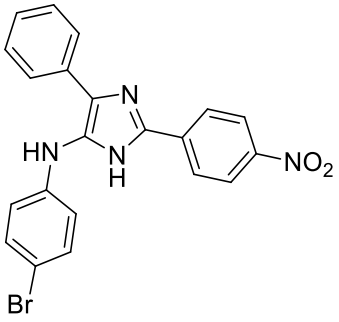
116.49, 110.47; ^{19}F NMR (376 MHz, CD_3OD): δ -114.66. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_3BrF$ 408.0512; found 408.0497.

***N*-(4-Bromophenyl)-5-phenyl-2-[4-(trifluoromethyl)phenyl]-1*H*-imidazol-5-amine (4am).**



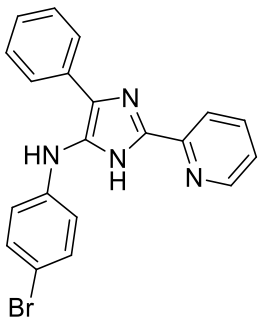
Purification by silica gel column chromatography (0 to 25% EtOAc in *n*-hexane) afforded **4am** as white solid (0.43 g, yield 93%), mp 215−217 ℃. ^{1}H NMR (400 MHz, CD_3OD): δ 8.12 (d, *J* = 8.0 Hz, 2H), 7.75 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.25 (t, *J* = 7.2 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 2H), 6.68 (d, *J* = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 147.44, 143.79, 134.82, 132.81, 131.32, 131.00, 129.68, 128.25, 127.13, 126.91, 126.83, 126.80, 124.26, 116.59, 110.63; ^{19}F NMR (376 MHz, CD_3OD): δ -64.20. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{22}H_{16}N_3BrF_3$ 458.0480; found 458.0473.

***N*-(4-Bromophenyl)-2-(4-nitrophenyl)-5-phenyl-1*H*-imidazol-5-amine (4an).**



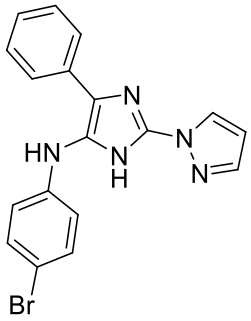
Purification by silica gel column chromatography (0 to 13% EtOAc in *n*-hexane) afforded **4an** as brown solid (0.15 g, yield 35%), mp 236−239 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 8.32 (d, J = 8.4 Hz, 2H), 8.16 (d, J = 8.4 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 7.38 (t, J = 8.0 Hz, 2H), 7.27 (t, J = 8.0 Hz, 2H), 7.22 (d, J = 8.4 Hz, 2H), 6.70 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 146.45, 144.97, 140.69, 134.75, 130.57, 127.48, 126.18, 124.98, 124.75, 122.95, 114.44, 108.52. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{21}H_{16}N_4O_2Br$ 435.0457; found 435.0438.

_N_-(4-Bromophenyl)-5-phenyl-2-(pyridin-2-yl)-1_H_-imidazol-5-amine (4ao).



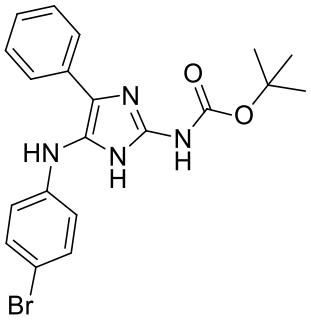
Purification by silica gel column chromatography (0 to 40% EtOAc in *n*-hexane) afforded **4ao** as brown solid (0.11 g, yield 30%), mp 155−157 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 8.63 (d, J = 4.0 Hz, 1H), 8.04 (d, J = 7.6 Hz, 1H), 7.86 (td, J = 8.0 Hz, 1.6 Hz, 1H), 7.74 (d, J = 7.6 Hz, 2H), 7.38−7.34 (m, 3H), 7.24 (t, J = 7.6 Hz, 1H), 7.21 (d, J = 8.8 Hz, 2H), 6.68 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, CD_3OD): δ 149.00, 147.96, 146.05, 142.99, 137.14, 131.46, 128.37, 126.92, 125.77, 123.20, 119.83, 115.29, 115.12, 109.18. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{20}H_{16}N_4Br$ 391.0558; found 391.0545.

_N_-(4-Bromophenyl)-5-phenyl-2-(1_H_-pyrazol-1-yl)-1_H_-imidazol-5-amine (4ap).



Purification by silica gel column chromatography (0 to 20% EtOAc in *n*-hexane) afforded **4ap** as white solid (0.12 g, yield 30%), mp 236−239 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 8.25 (d, J = 2.0 Hz, 1H), 7.76 (s, 1H), 7.70 (d, J = 7.6 Hz, 2H), 7.34 (d, J = 7.6 Hz, 2H), 7.24−7.20 (m, 3H), 6.67 (d, J = 8.8 Hz, 2H), 6.53 (t, J = 2.0 Hz, 1H); ^{13}C NMR (100 MHz, CD_3OD): δ 146.02, 141.56, 138.97, 131.41, 128.17, 127.68, 126.54, 125.46, 115.15, 109.31, 109.45. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{18}H_{15}N_5Br$ 380.0511; found 380.0502.

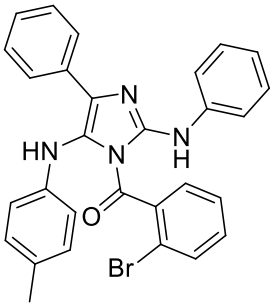
Tert-butyl {5-[(4-bromophenyl)amino]-4-phenyl-1*H*-imidazol-2-yl}carbamate (4aq).



Purification by silica gel column chromatography (0 to 35% EtOAc in *n*-hexane) afforded **4aq** as white solid (0.24 g, yield 63%), mp 236−239 °C. ^{1}H NMR (400 MHz, CD_3OD): δ 7.75 (d, J = 7.2 Hz, 2H), 7.29−7.23 (m, 4H), 7.20 (t, J = 7.2 Hz, 1H), 6.51 (d, J = 8.8 Hz, 2H), 1.35 (s, 9H); ^{13}C NMR (150 MHz, CD_3OD): δ 149.76, 148.89, 145.30, 133.42,

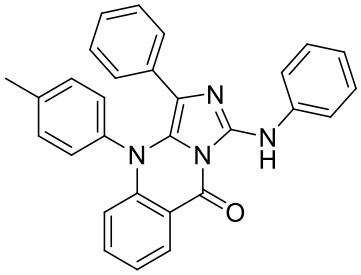
132.50, 132.09, 128.30, 127.37, 126.49, 117.13, 115.49, 111.26, 85.73, 27.82. HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{20}H_{22}N_4O_2Br$ 429.0926; found 429.0923.

(2-Bromophenyl)(4-phenyl-2-(phenylamino)-5-(*p*-tolylamino)-1*H*-imidazol-1-yl)methanone (5a).



TEA (0.76 g, 2.30 mmol) and 4-DMAP (0.02 g, 0.15 mmol) were added to a solution of **4a** (0.25 g, 0.77 mmol) in DCM: THF (4: 1) (15 mL) at 0 ℃ and stirred for 30 minutes. To this mixture 2-bromobenzoyl chloride (0.18 g, 0.85 mmol) was added drop wise and stirred for 16h slowly raising to rt. Reaction mass was diluted with water (30 mL) and extracted with EtOAc (2X50 mL). The combined organic layer was washed with brine (30 mL), dried over sodium sulfate and concentrated in *vacuo*. Purification by silica gel column chromatography (0 to 8% EtOAc in hexanes) afforded **5a** as yellow solid (0.20 g, yield 45%). mp 173–175 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, J = 8.8 Hz, 2H), 7.46 (dd, J = 8.0, 1.6 Hz, 2H), 7.32 (t, J = 7.2 Hz, 3H), 7.24–7.15 (m, 5H), 7.09– 7.06 (m, 2H), 6.91 (d, J = 8.8 Hz, 2H), 6.56 (d, J = 8.4 Hz, 2H), 6.16 (s, 1H), 2.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.47, 146.03, 141.03, 134.83, 133.78, 132.33, 132.30, 130.70, 130.46, 129.77, 129.46, 128.97, 128.63, 128.35, 128.25, 127.82, 126.41, 114.98, 114.64, 20.62; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{29}H_{23}BrN_3O$ 508.1024; found 508.1009.

3-Phenyl-1-(phenylamino)-4-(*p*-tolyl)imidazo[5,1-b]quinazolin-9(4*H*)-one (6a).

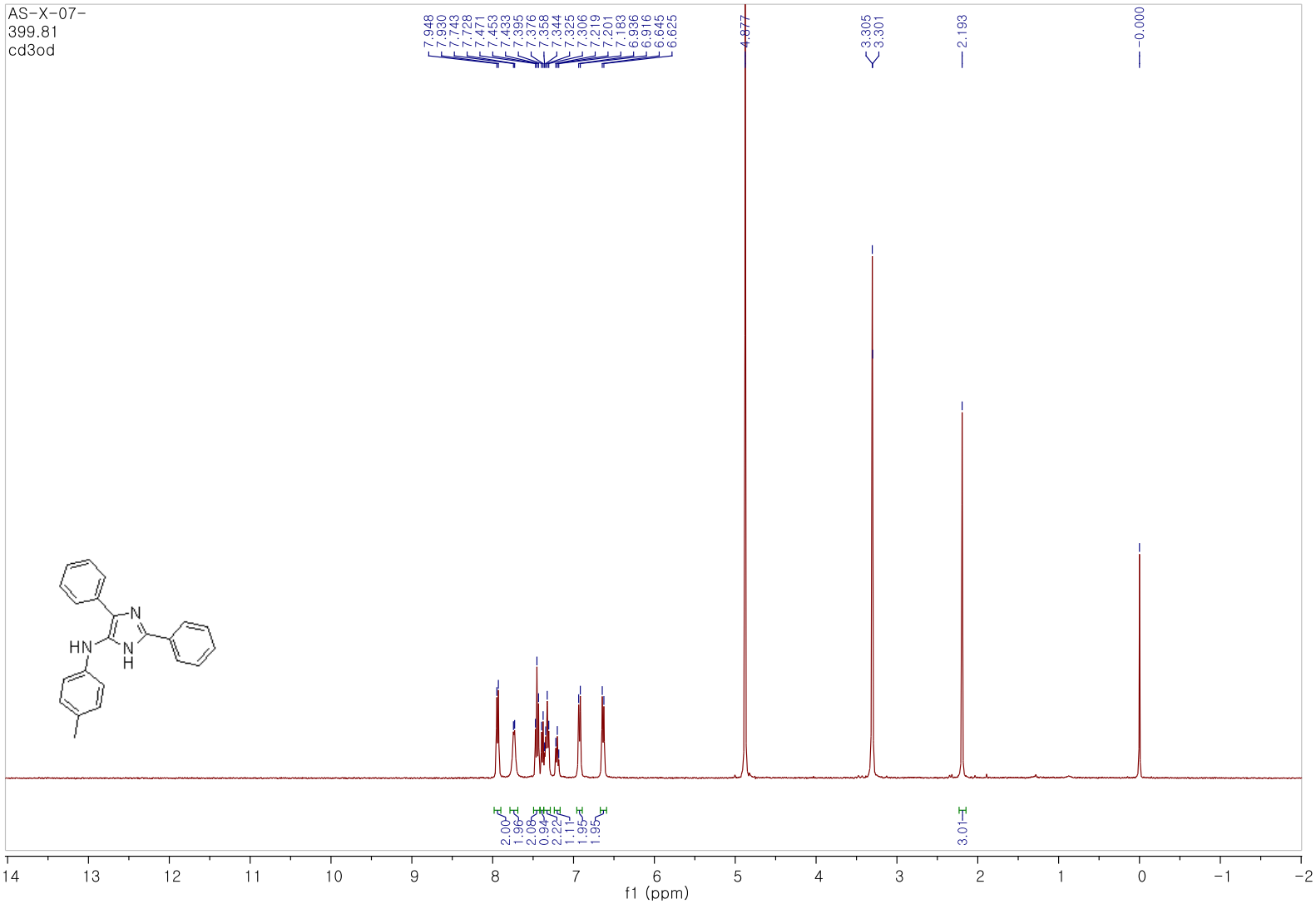


CuI (6.0 mg, 0.03 mmol) was added to a degassed solution of compound **5a** (200 mg, 0.34 mmol), K_2CO_3 (143 mg, 1.04 mmol), and (*trans*-N,N' -dimethylcyclohexane-1,2-diamine (10.0 mg, 0.07 mmol) in 1,4-dioxane (10 ml) and reaction mixture was stirred at 110℃ for 16h. Reaction mass was cooled to rt, diluted with water (30 mL) and extracted with EtOAc (2X50 mL). The combined organic layer was washed with brine (30 mL), dried over sodium sulfate and concentrated in *vacuo*. Purification by silica gel column chromatography (0 to 5% EtOAc in hexanes) afforded **6a** as yellow solid (95 mg, yield 65%). mp 227–230 ℃. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.36 (d, J = 7.2 Hz, 1H), 7.78(dd, J = 8.4, 2.0 Hz, 2H), 7.50–7.43 (m, 4H), 7.15 (t, J = 7.2 Hz, 1H), 7.06– 6.95 (m, 9H), 6.83 (d, J = 8.4 Hz, 1H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.49, 142.70, 139.31, 139.07, 135.15, 134.02, 133.87, 131.83, 130.30, 130.28, 129.87, 129.38, 129.28, 129.21, 128.53, 127.36, 126.99, 125.86, 121.48, 120.94, 21.03; HRMS (ESI) *m/z*: $[M + H]^+$ calcd for $C_{29}H_{22}N_3O$ 428.1763; found 428.1763.

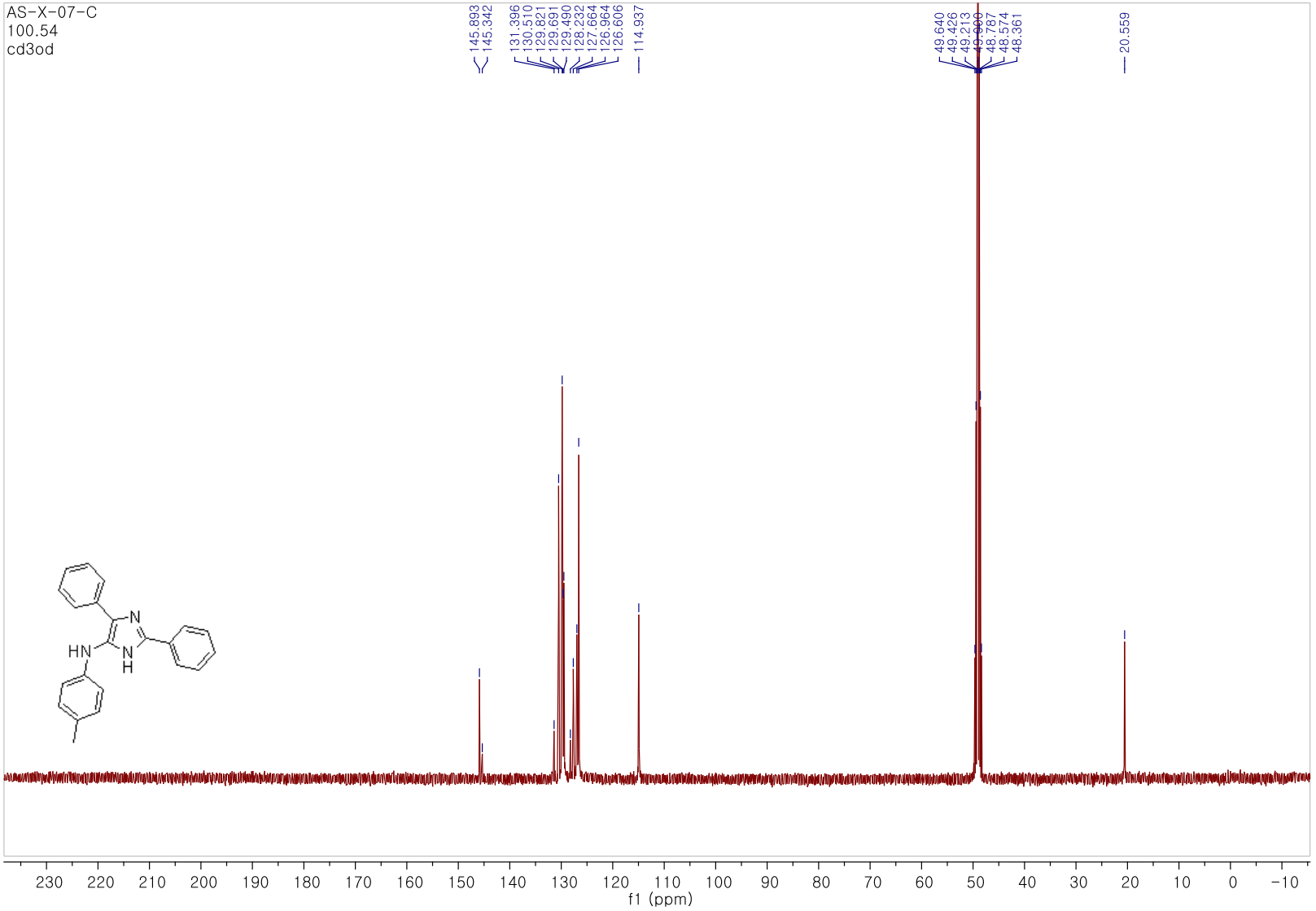
Abbreviations

DCM, dichloromethane; TEA, triethylamine; 4-DMAP, 4-(dimethylamino)pyridine; MeOH, methanol; THF, tetrahydrofuran; EtOAc, ethyl acetate; HRMS, high-resolution mass spectrometry; mp, melting point.

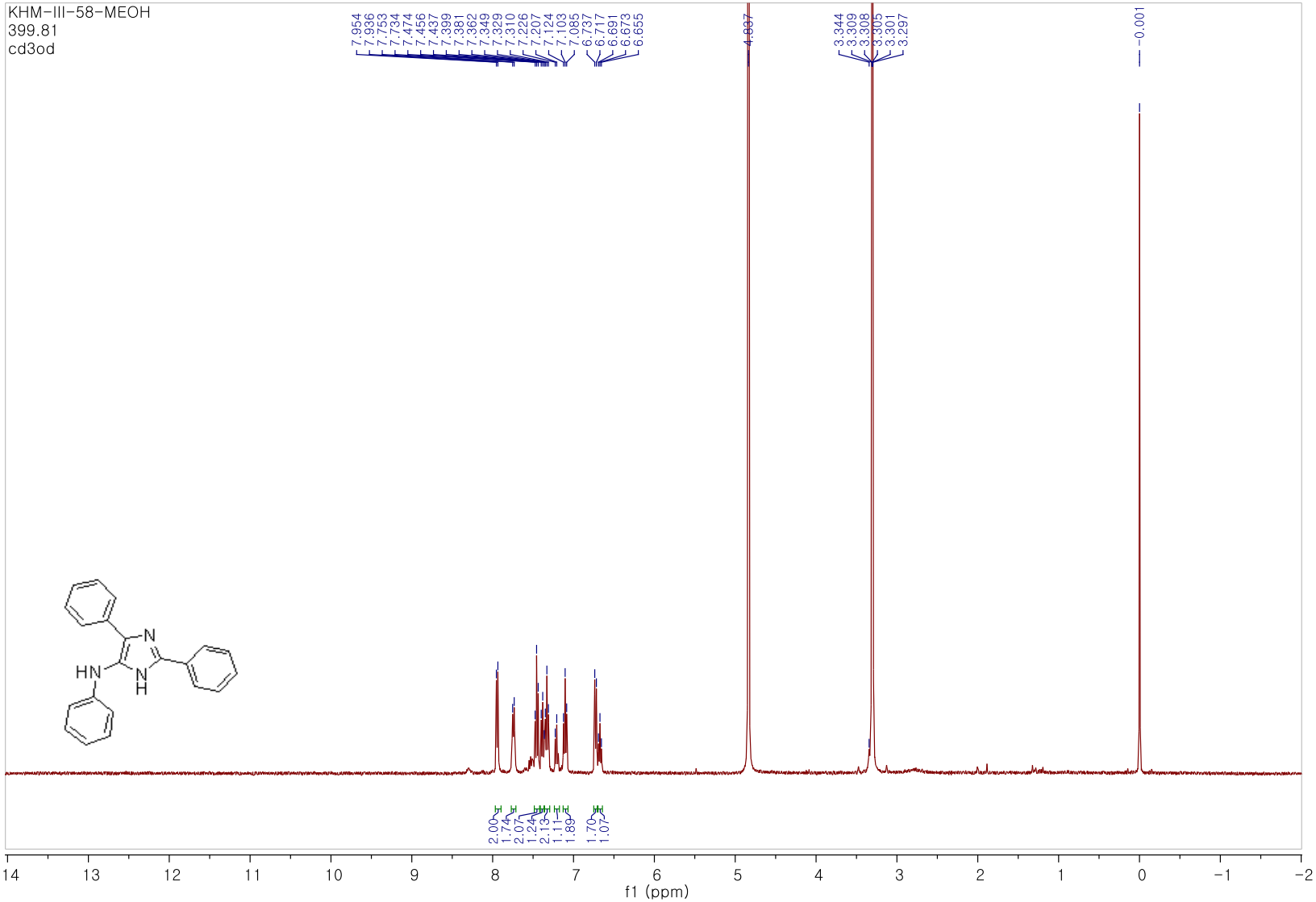
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4a**



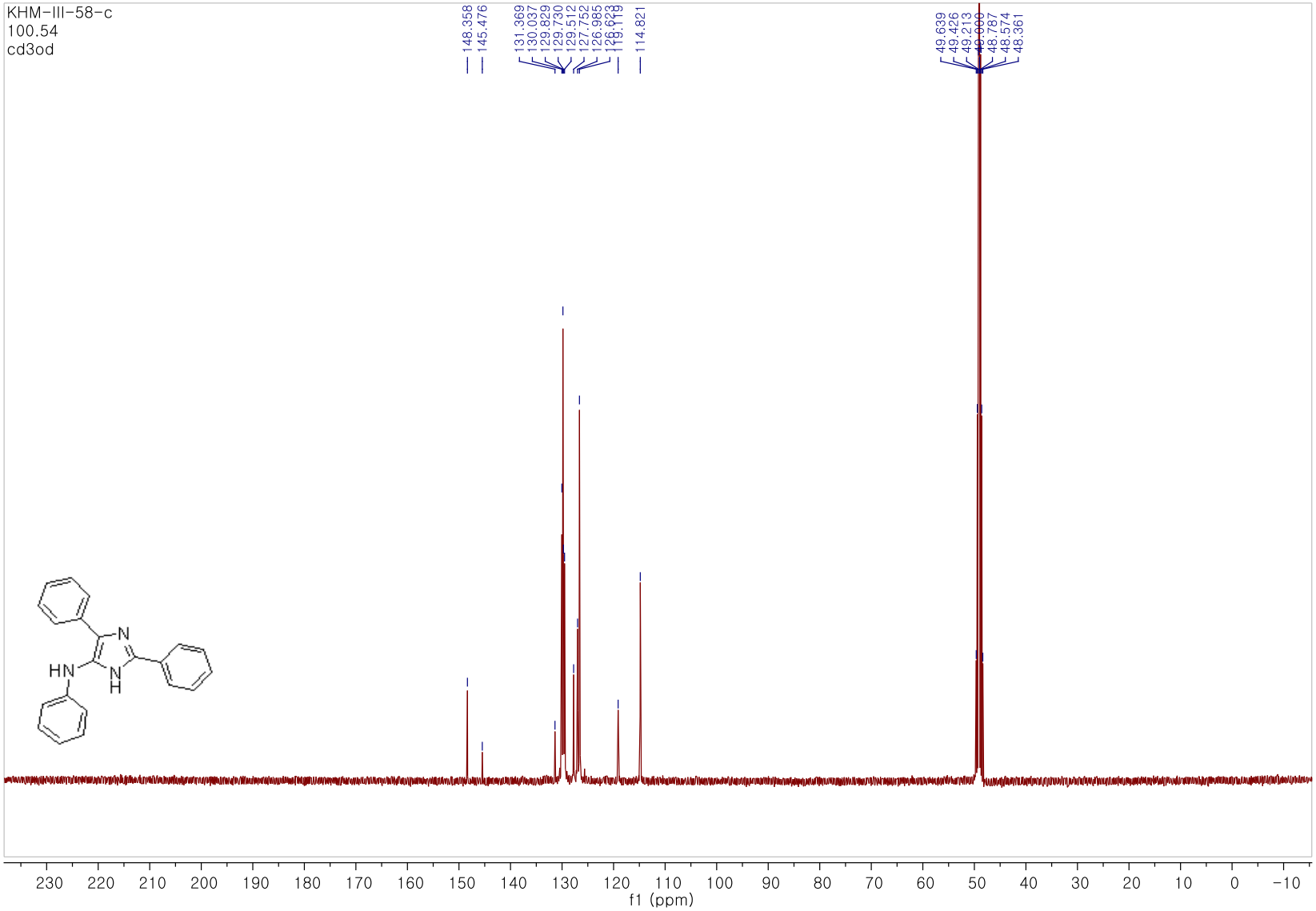
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4a**



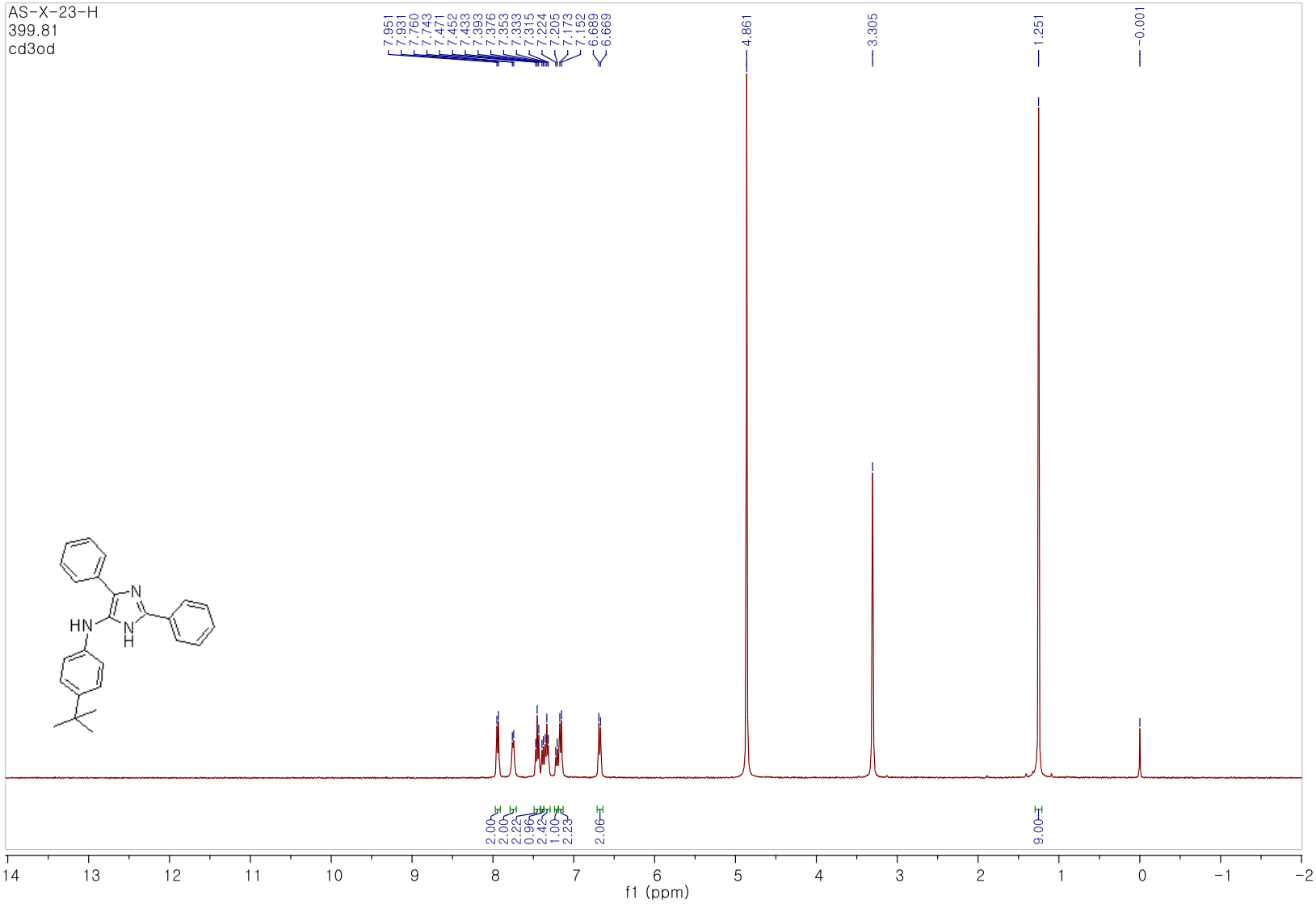
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4b**



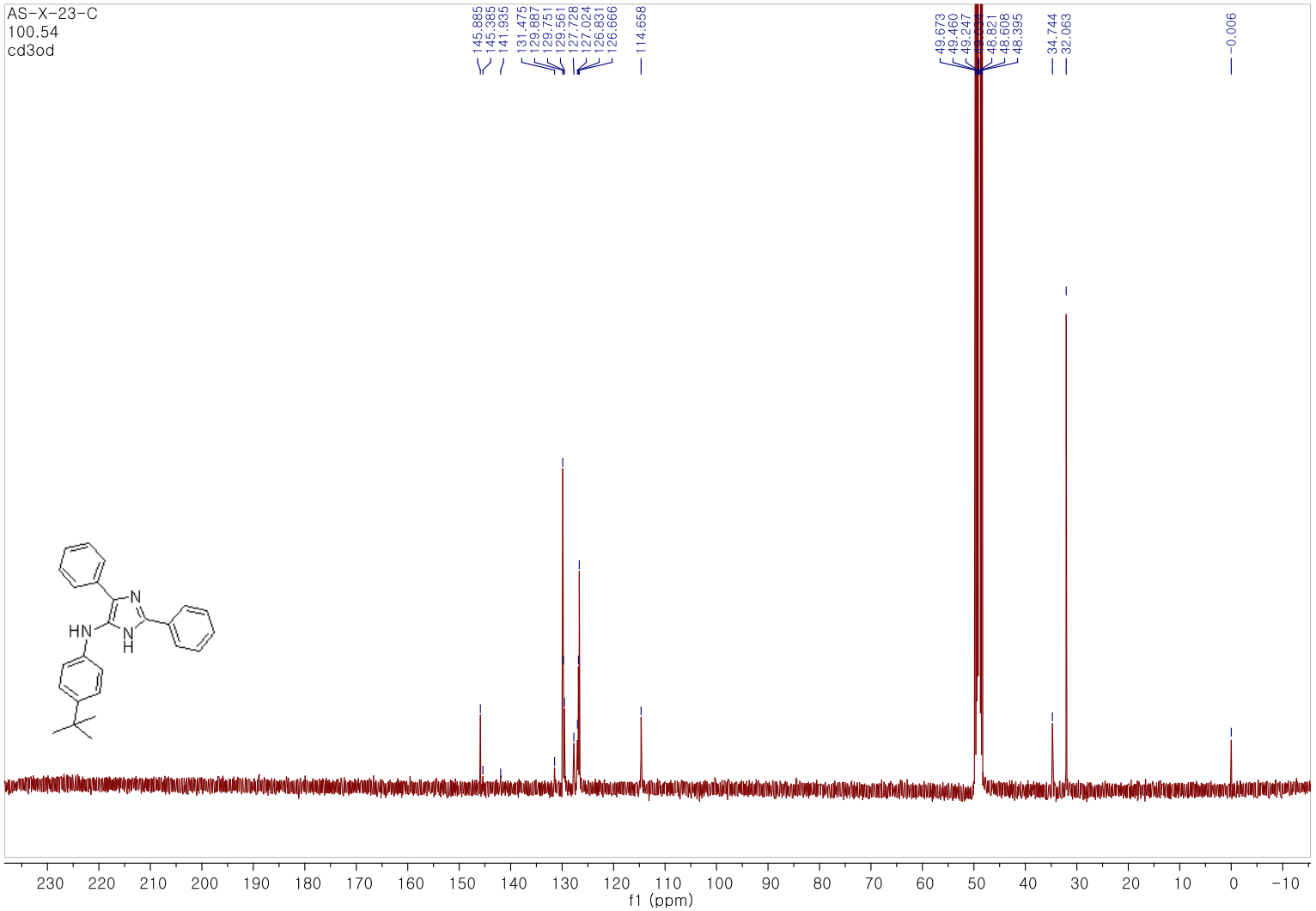
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4b**



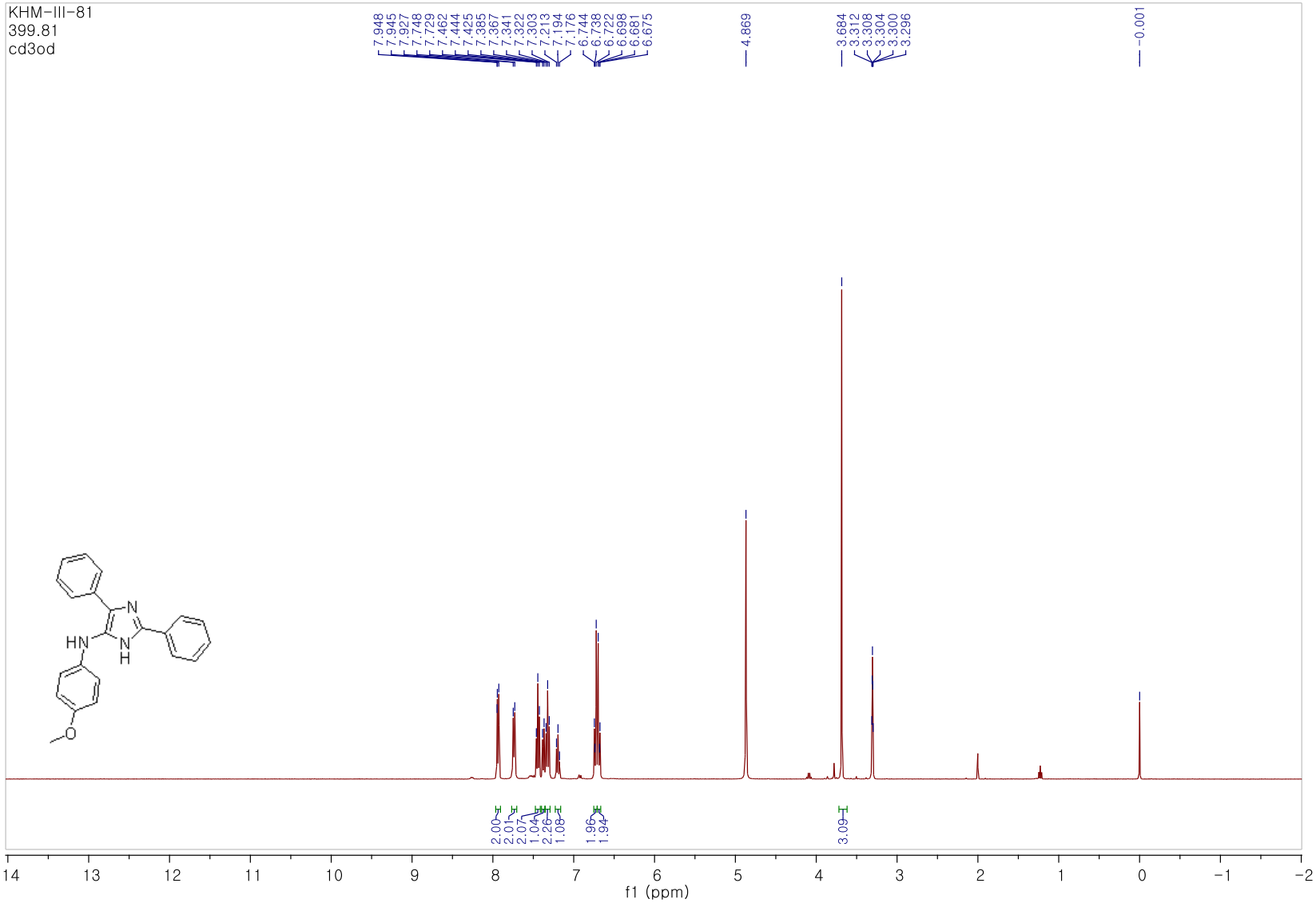
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4c**



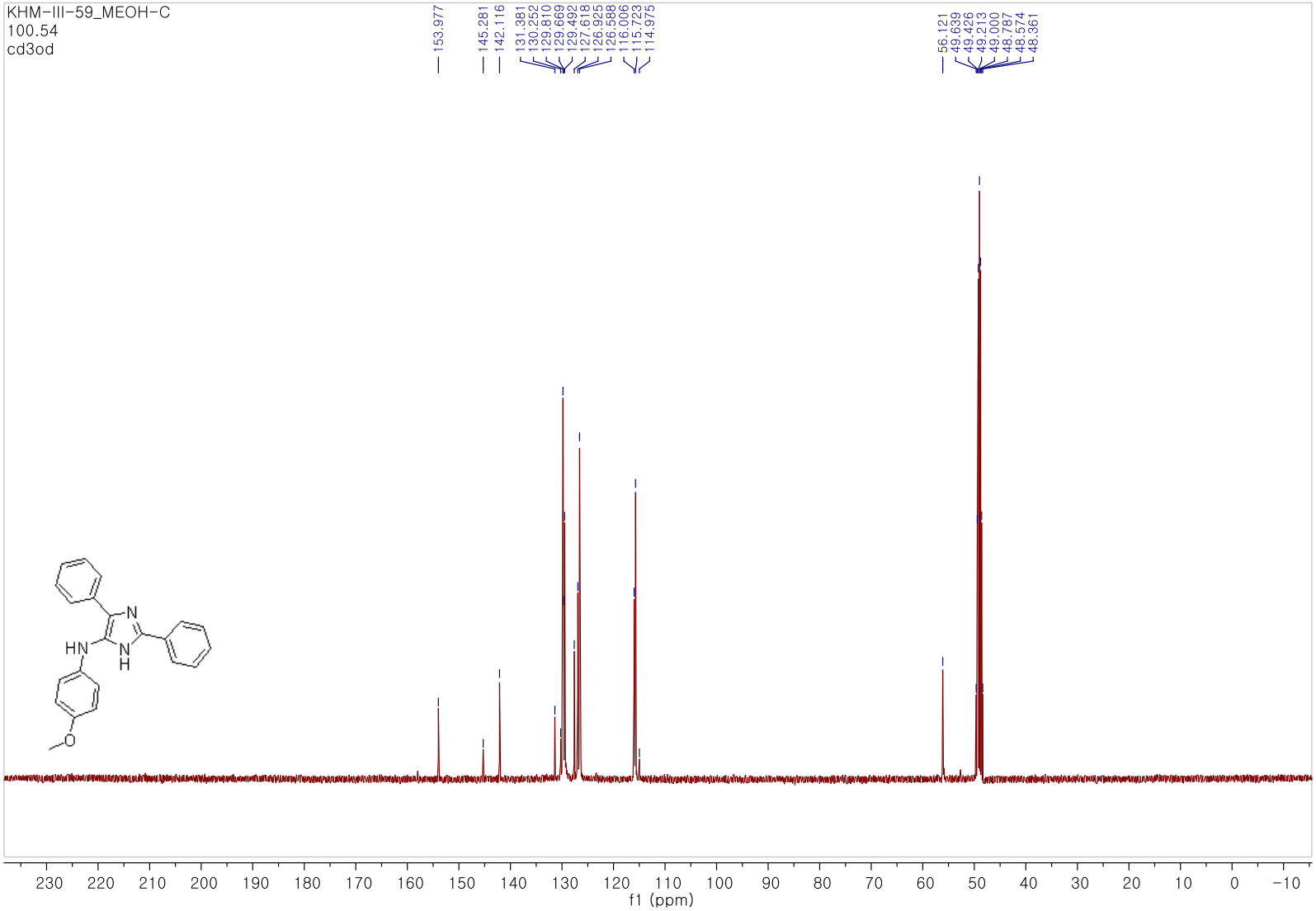
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4c**



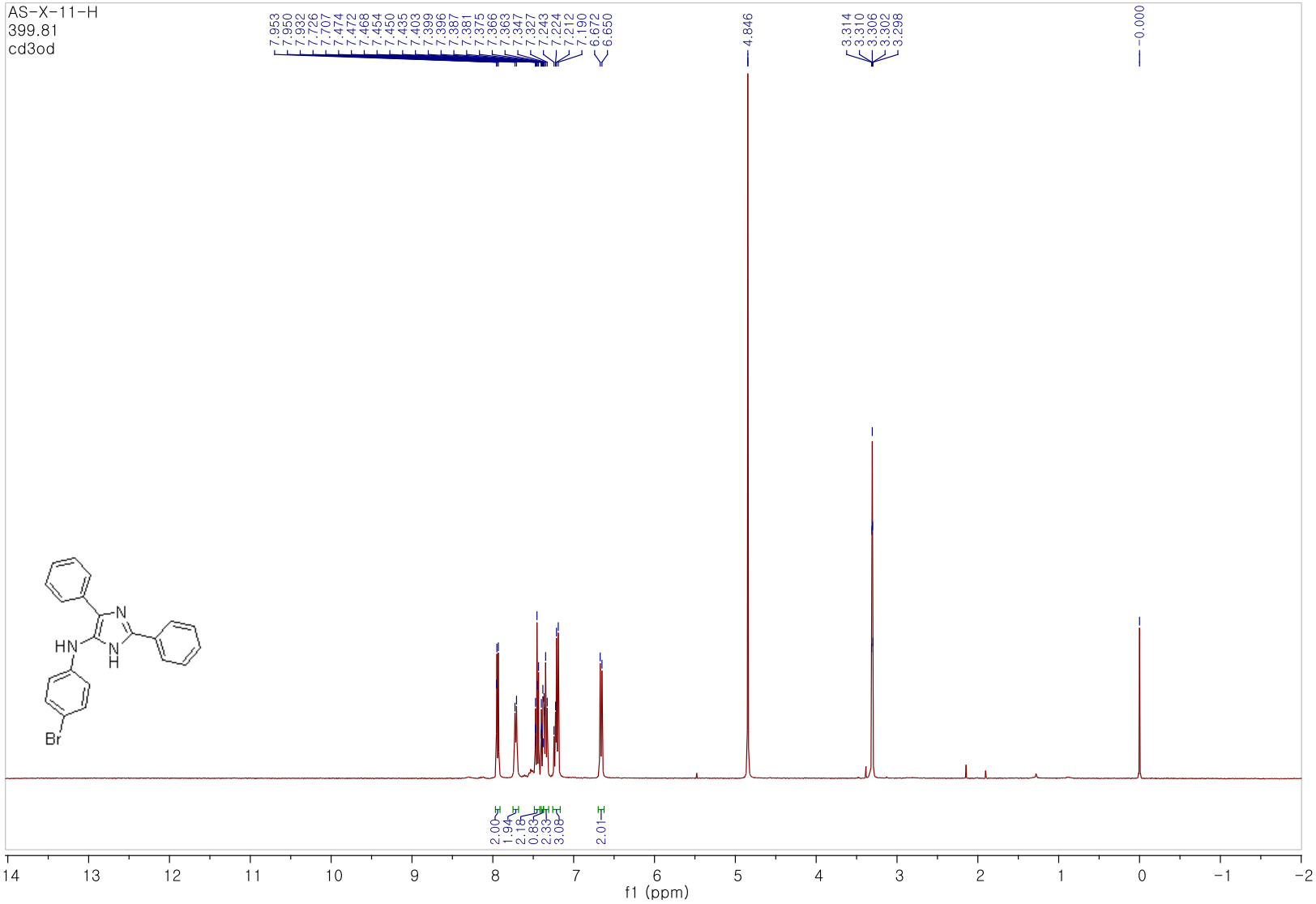
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4d**



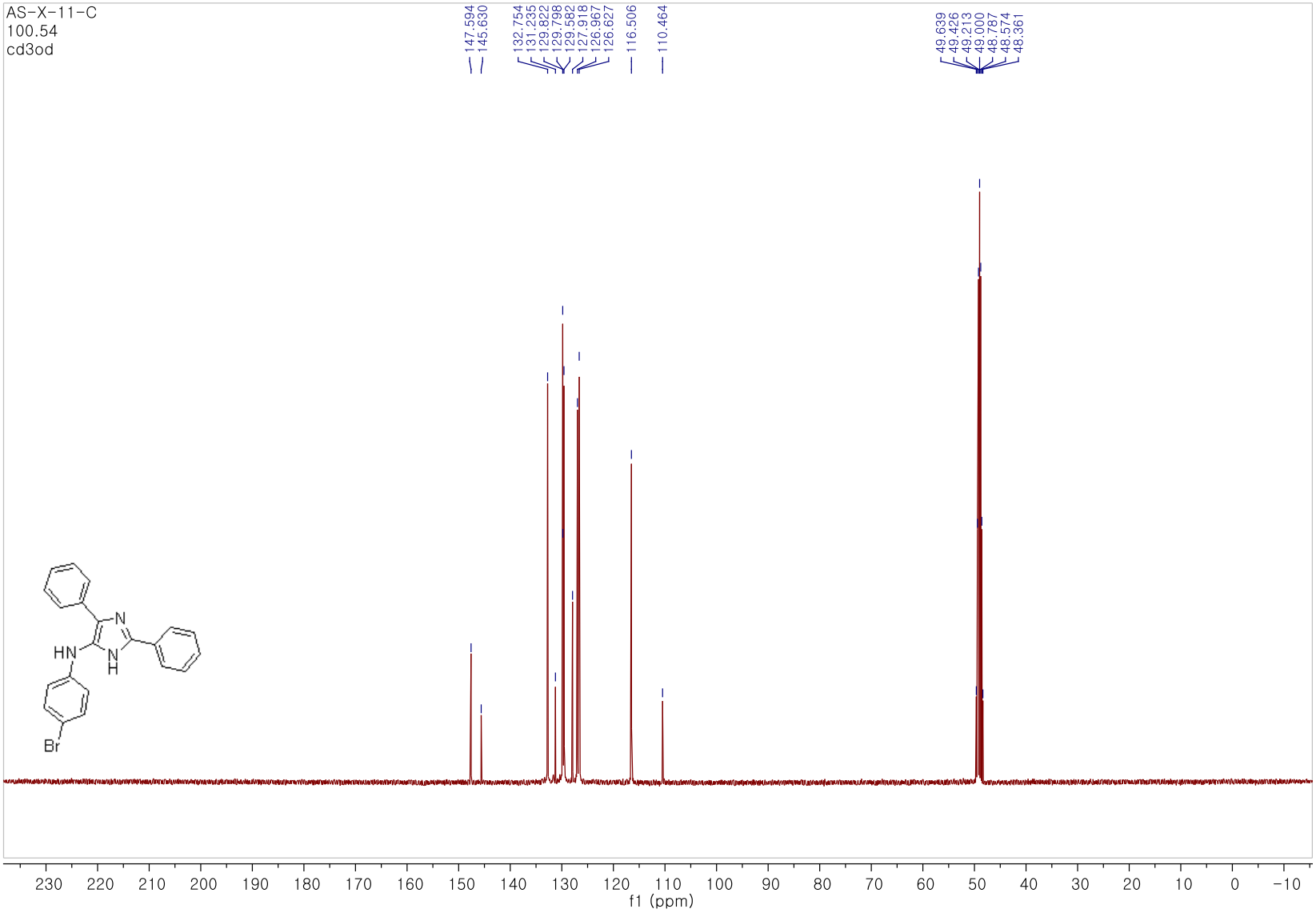
^{3}C NMR (100 MHz, methanol-d_4) spectrum of **4d**



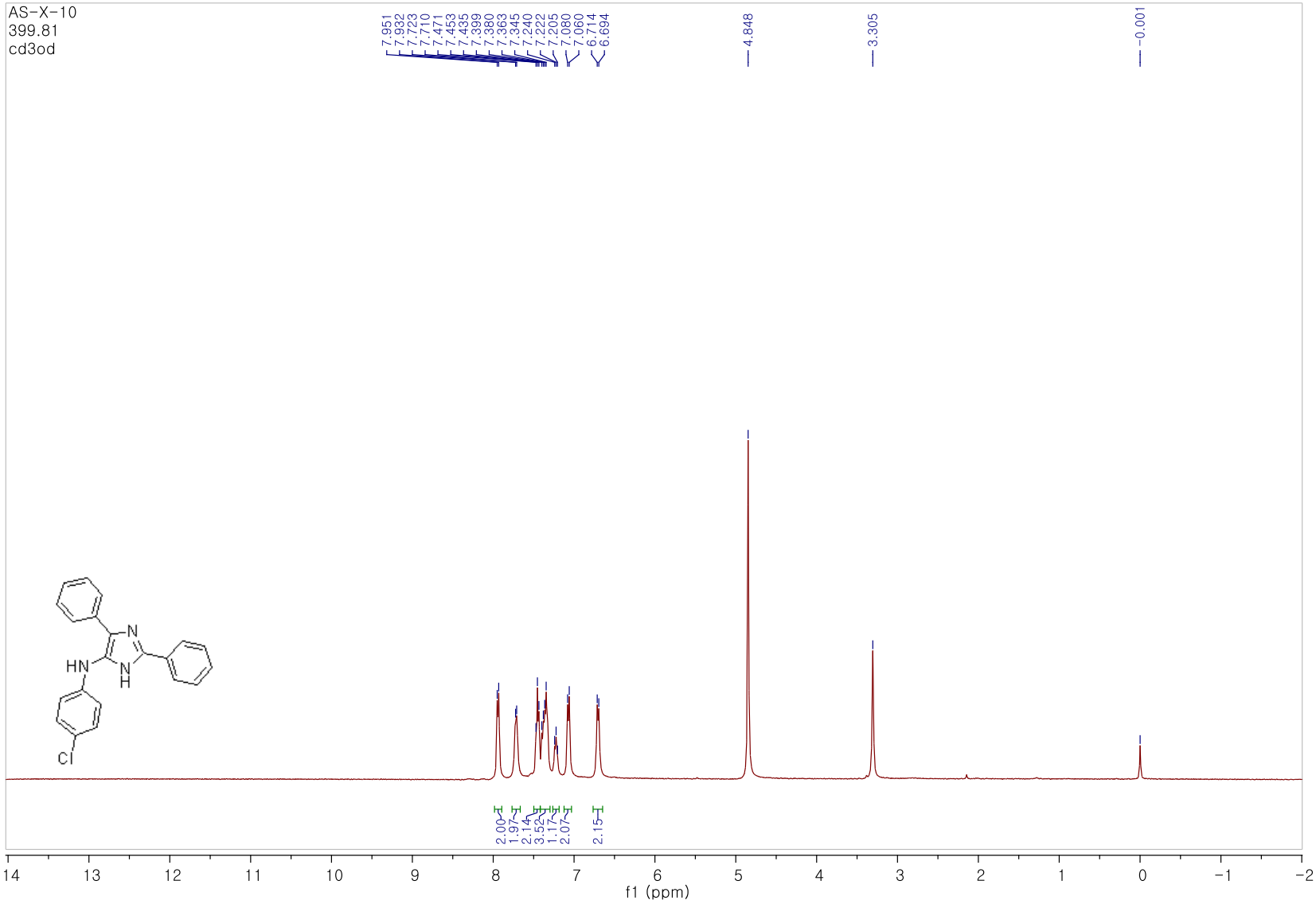
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4e**



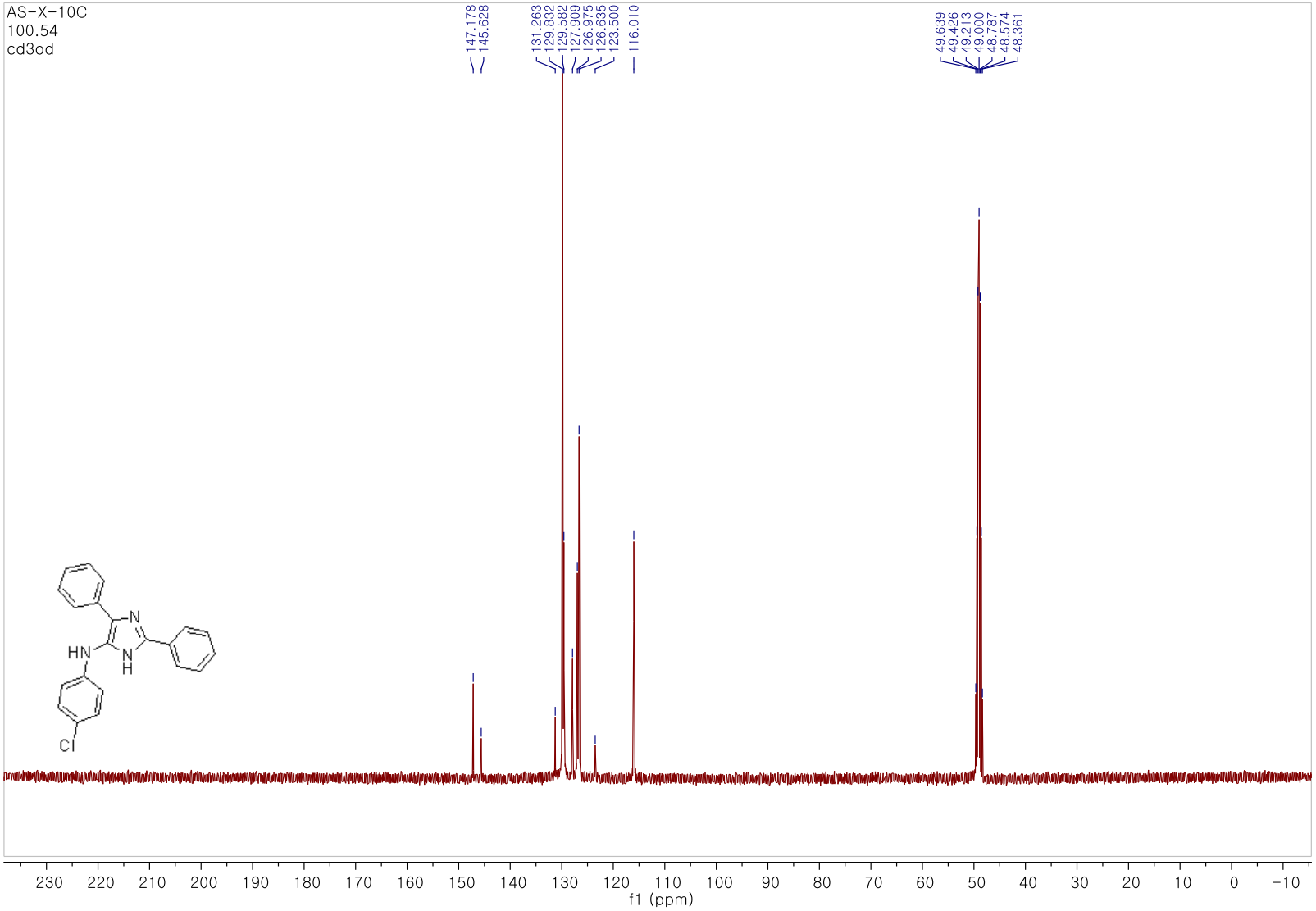
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4e**



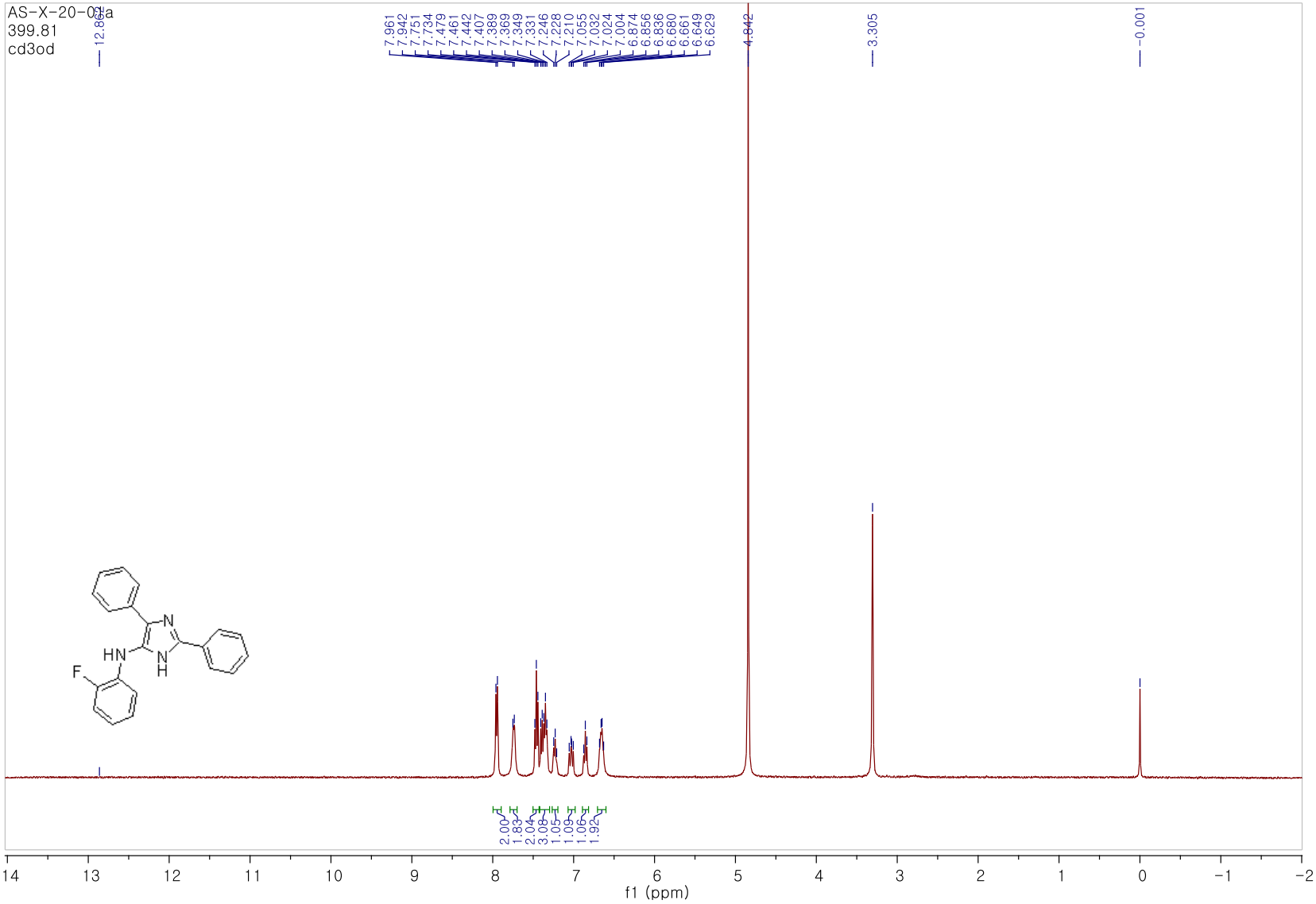
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4f**



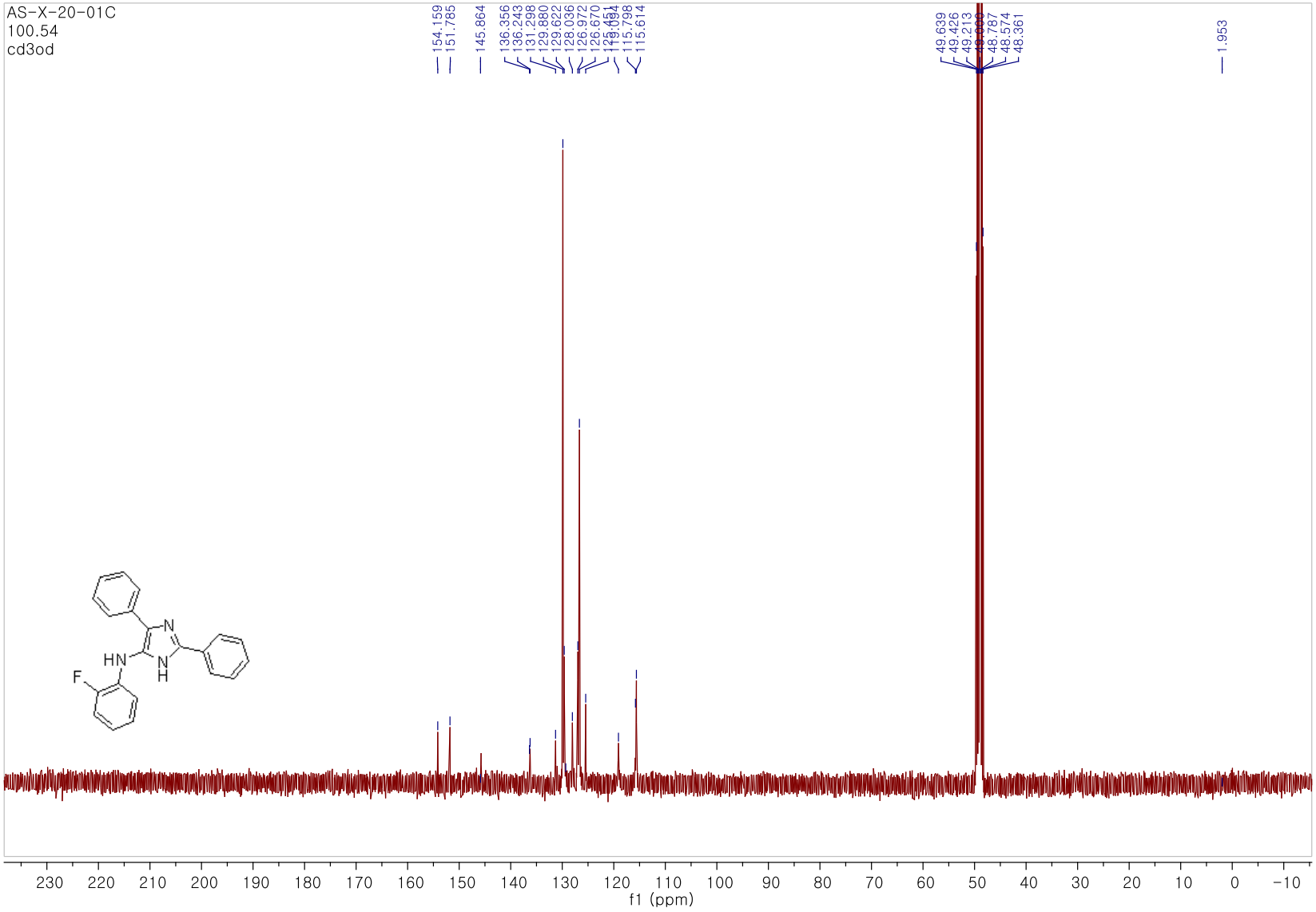
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4f**



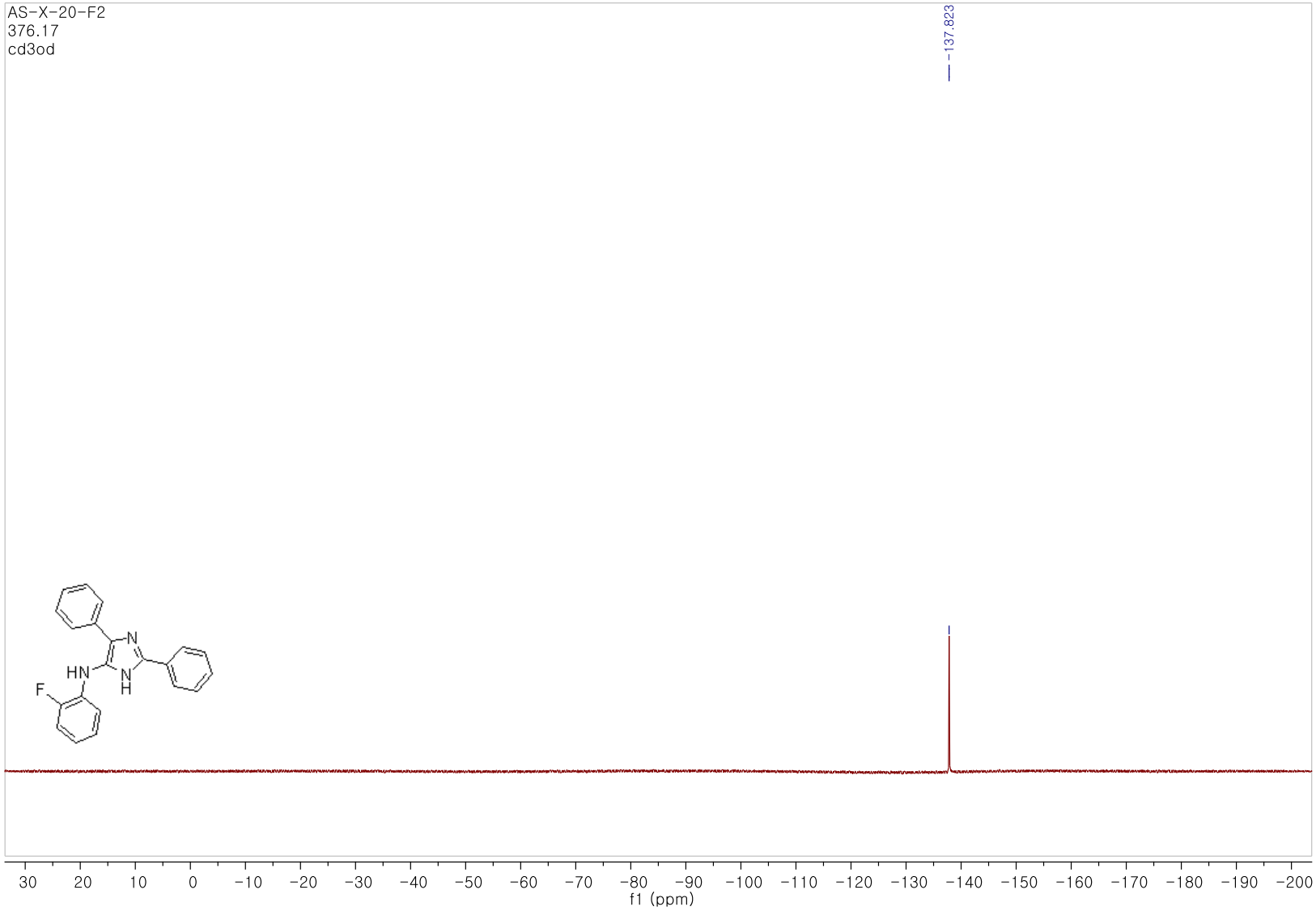
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4g**



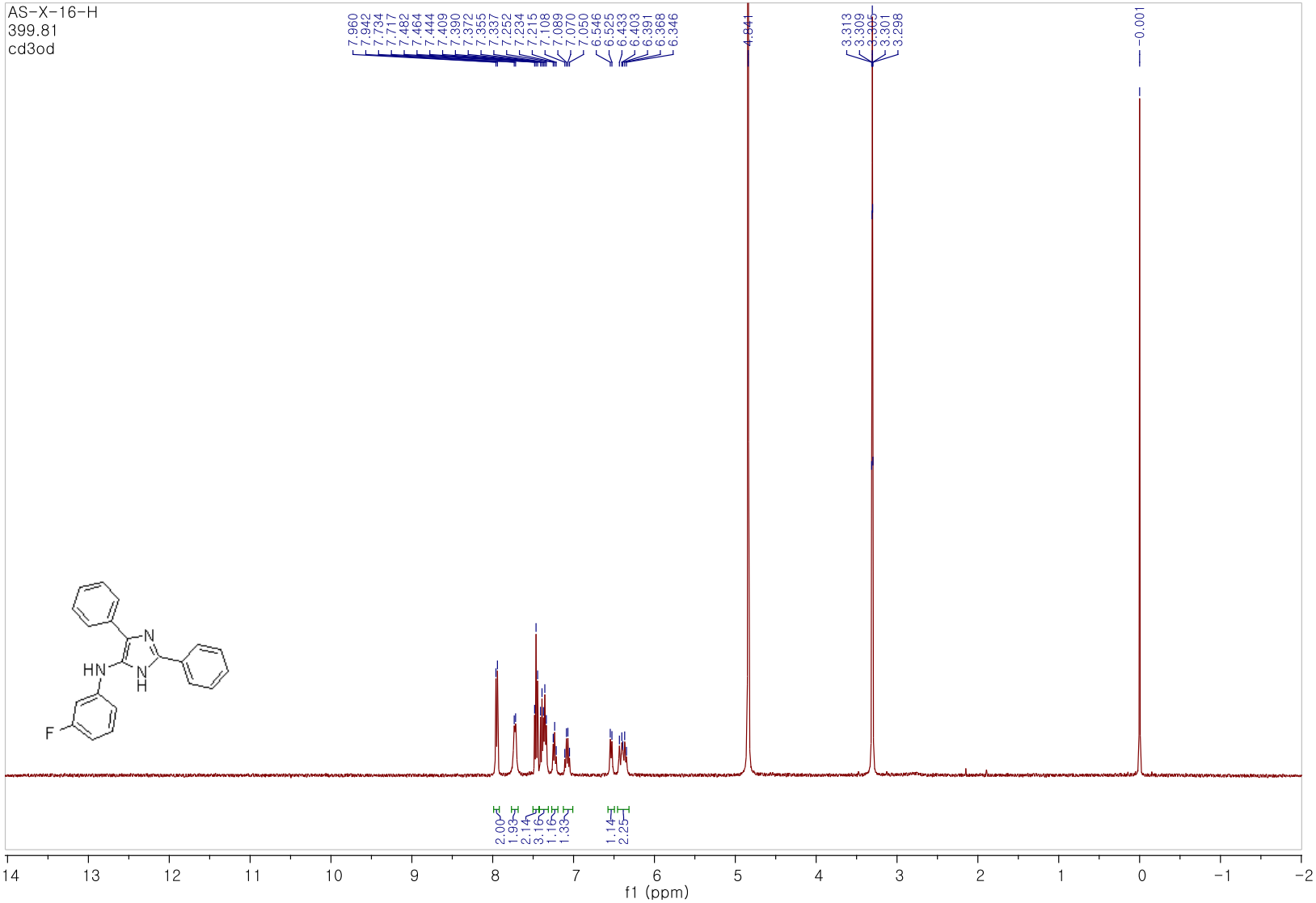
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4g**



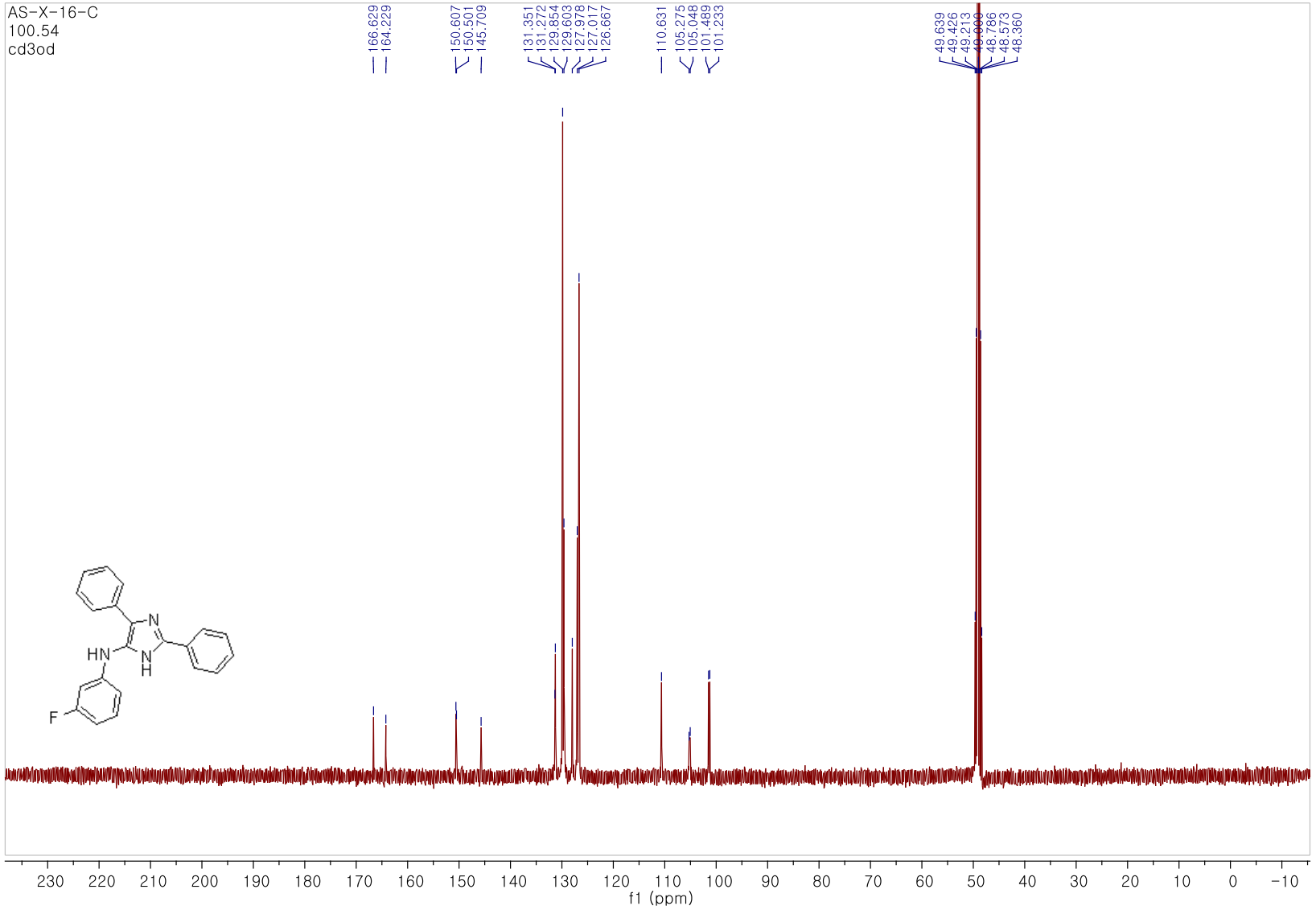
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4g**



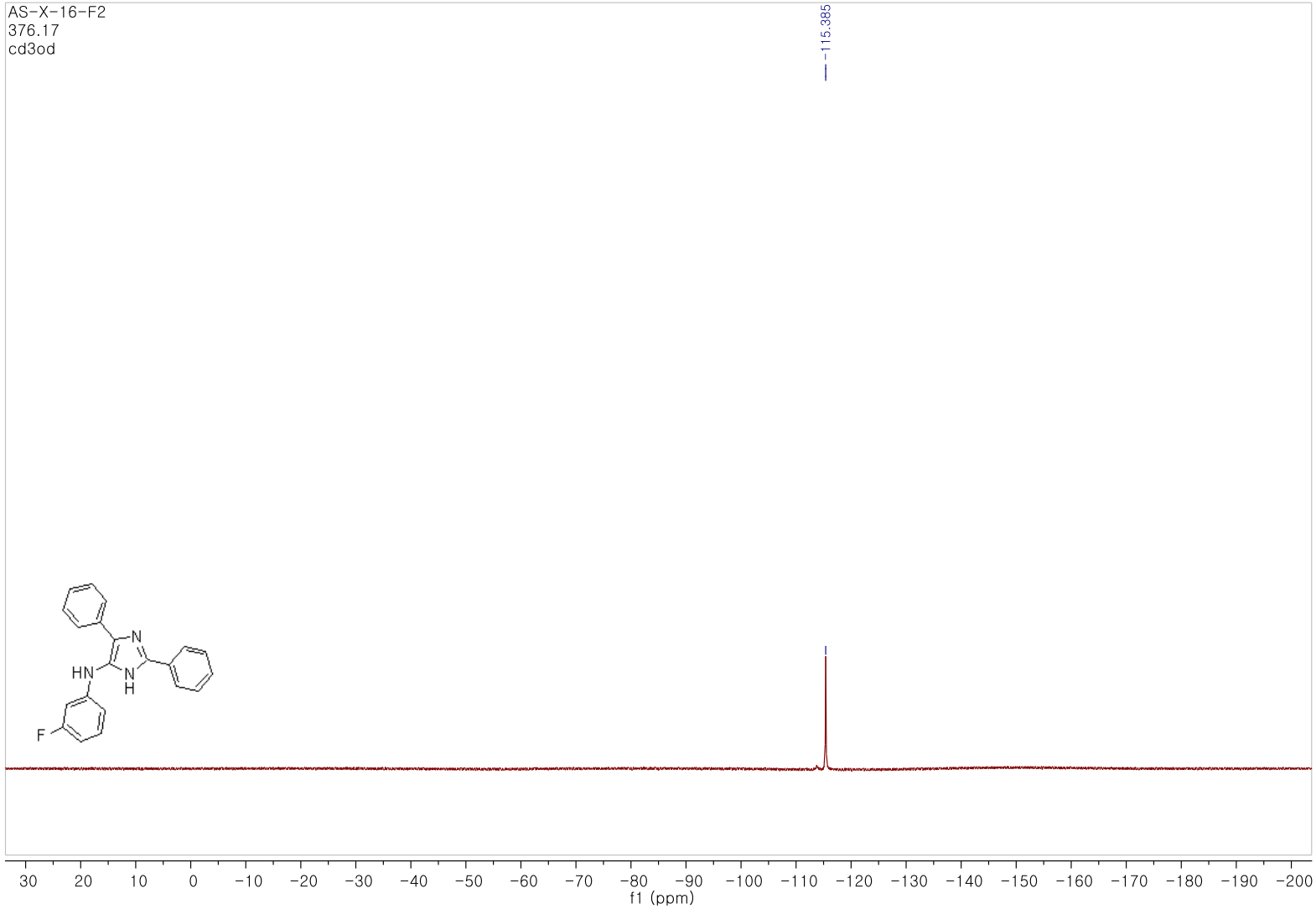
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4h**



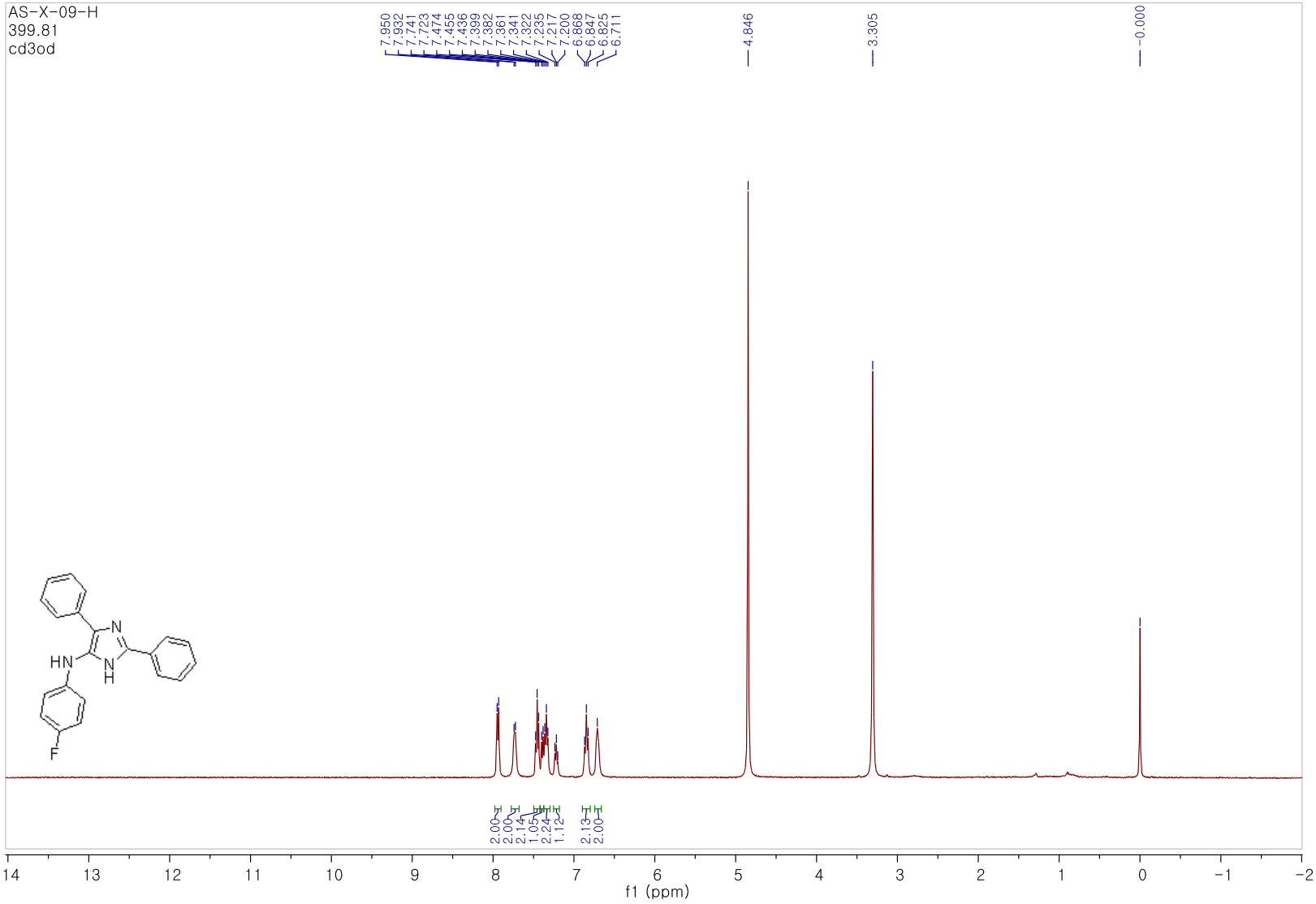
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4h**



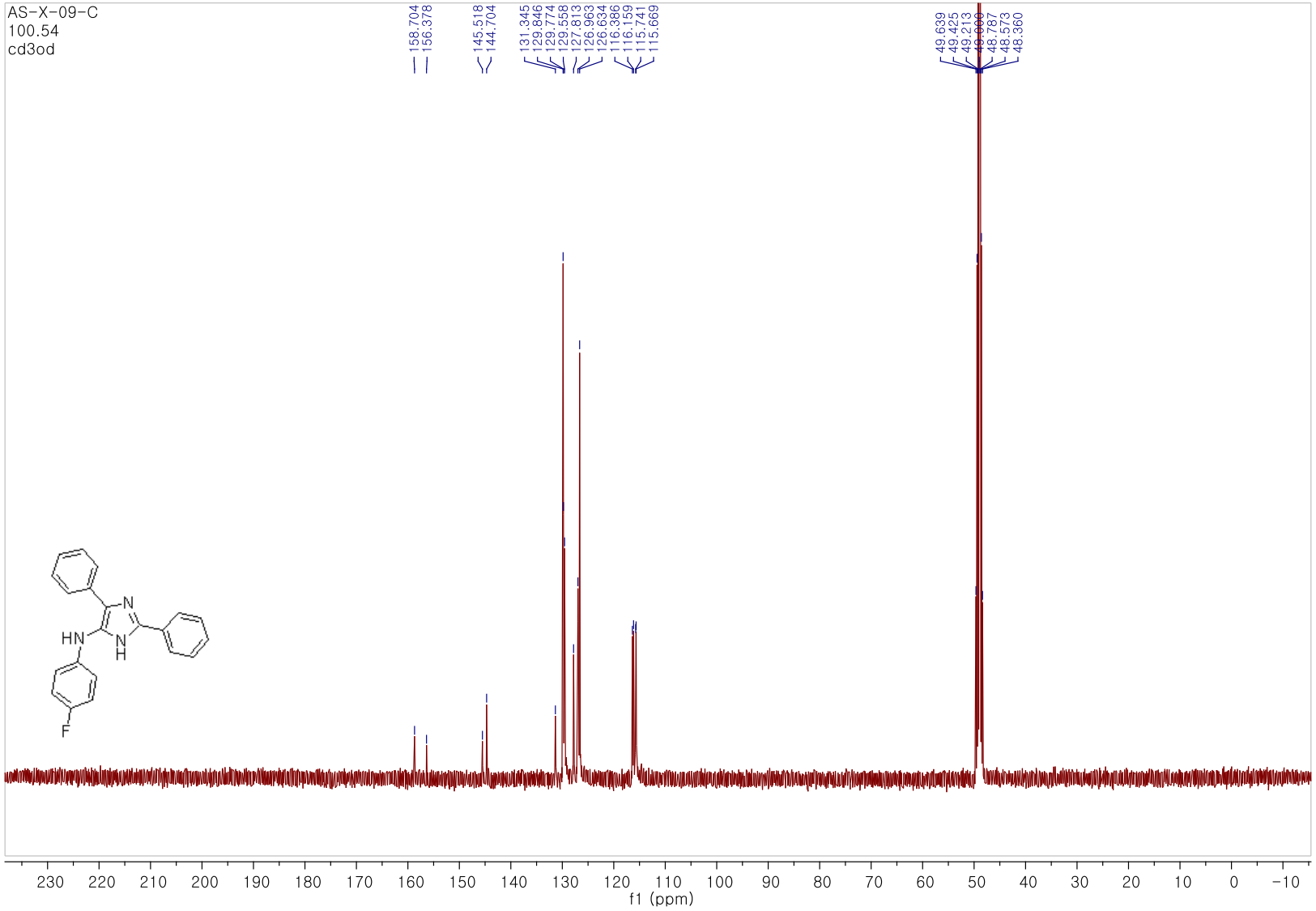
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4h**



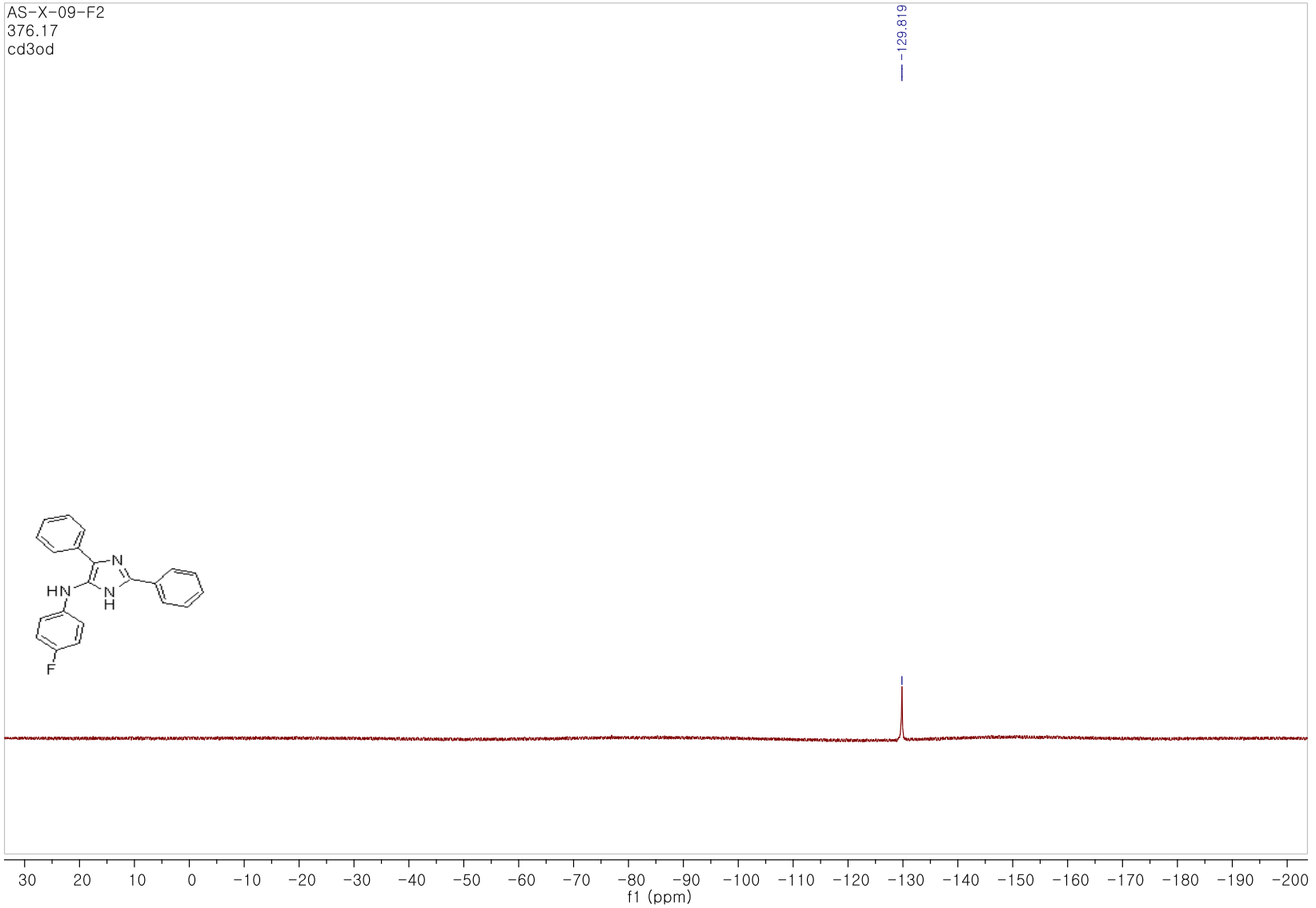
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4i**



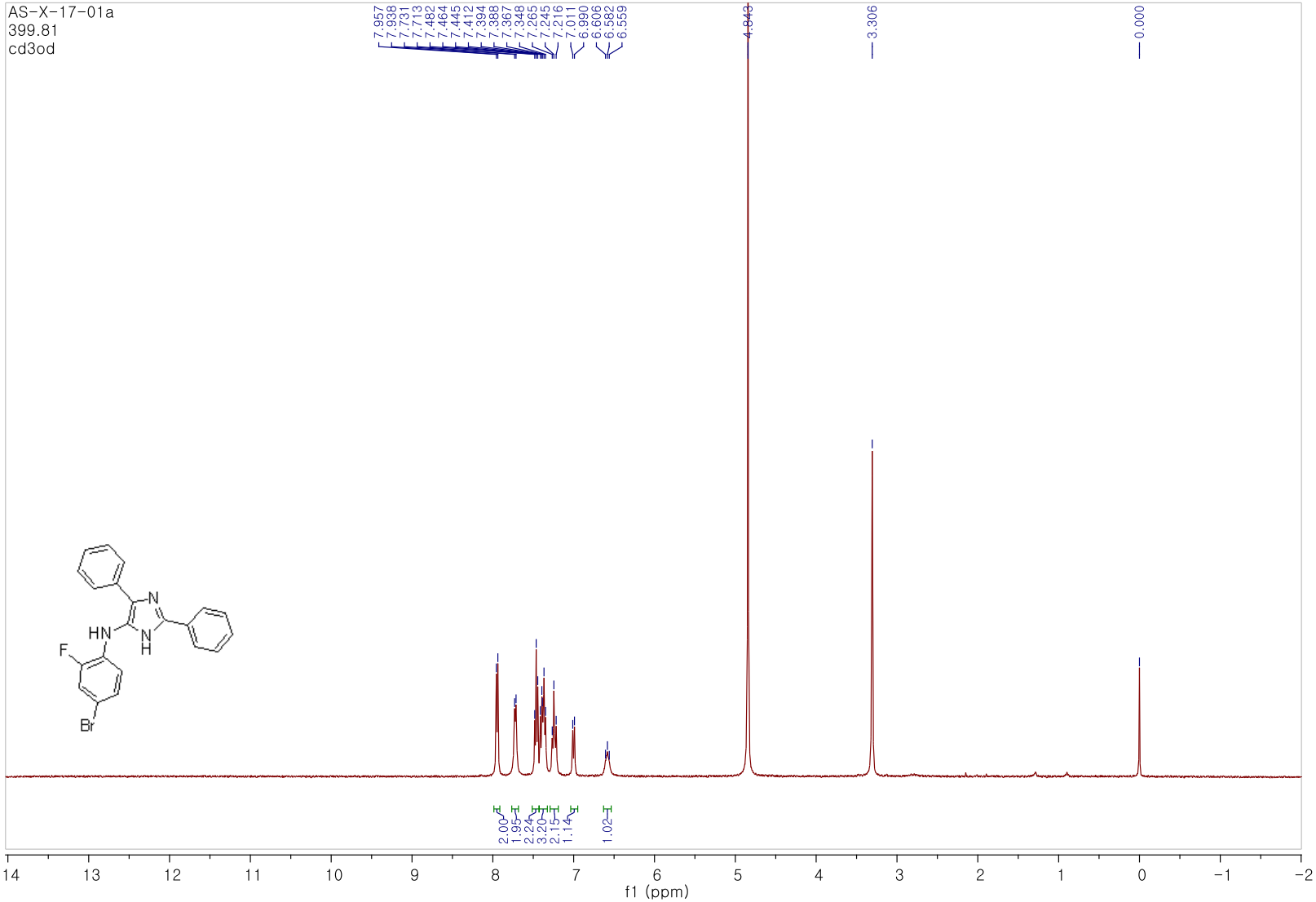
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4i**



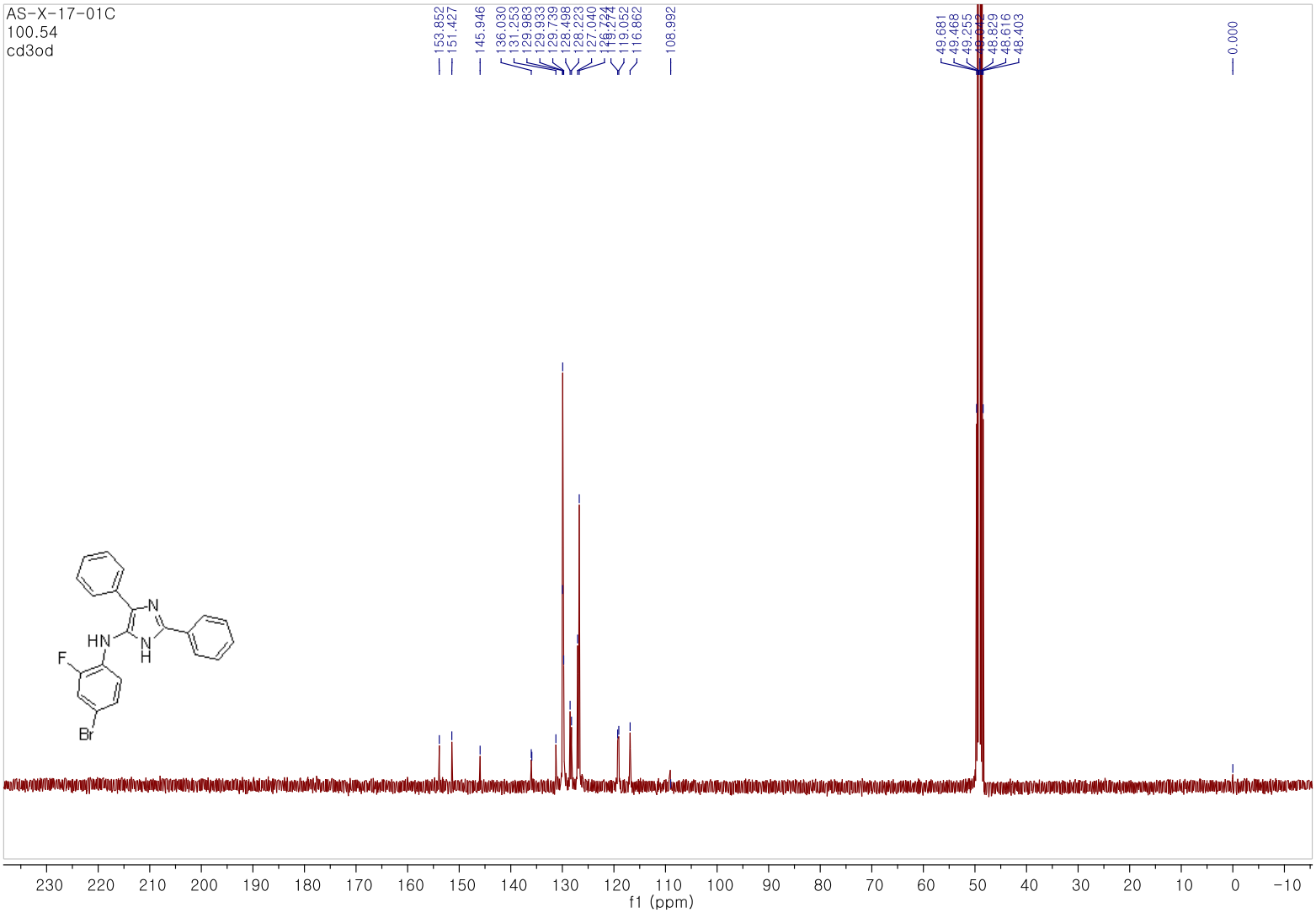
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4i**



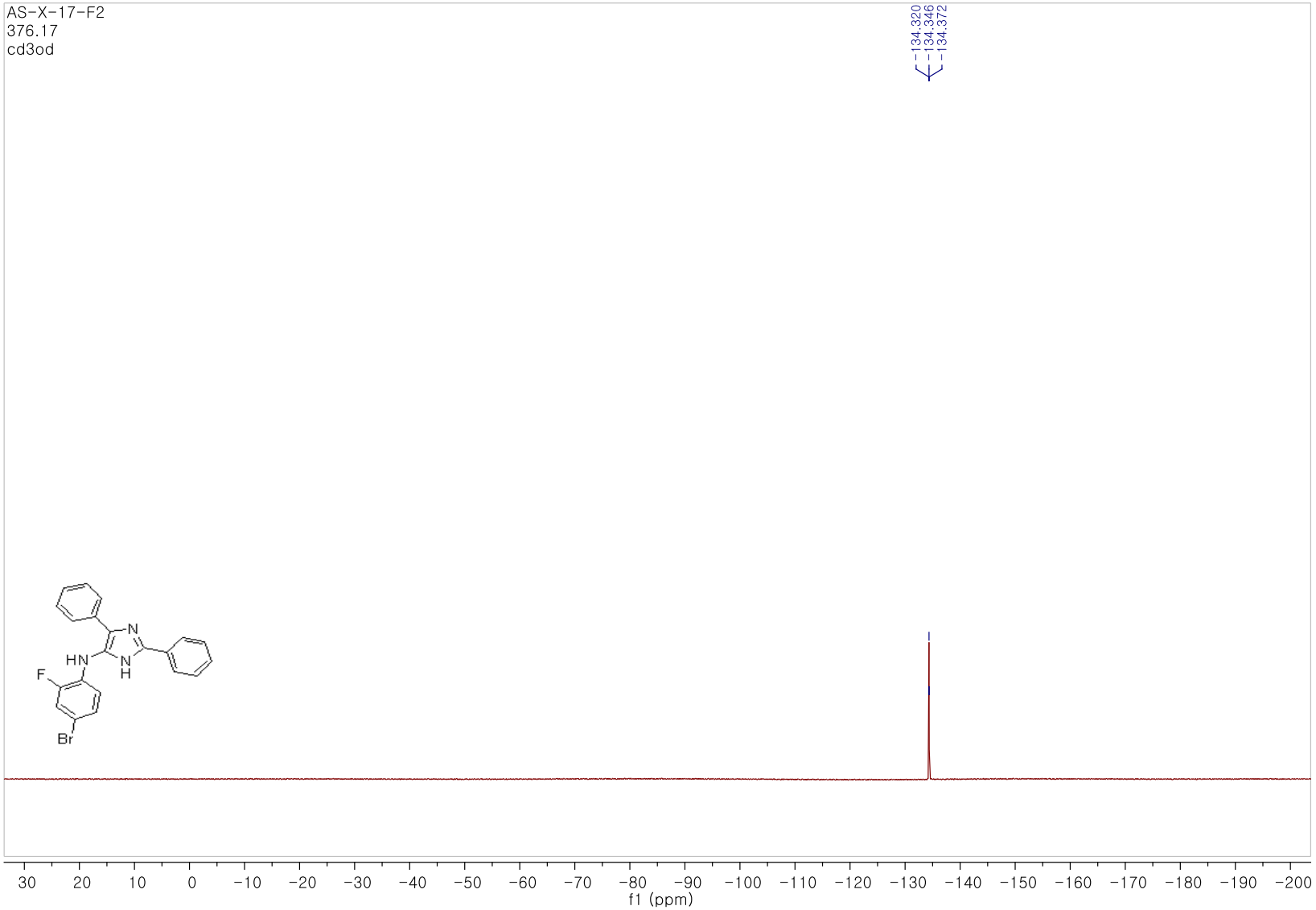
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4j**



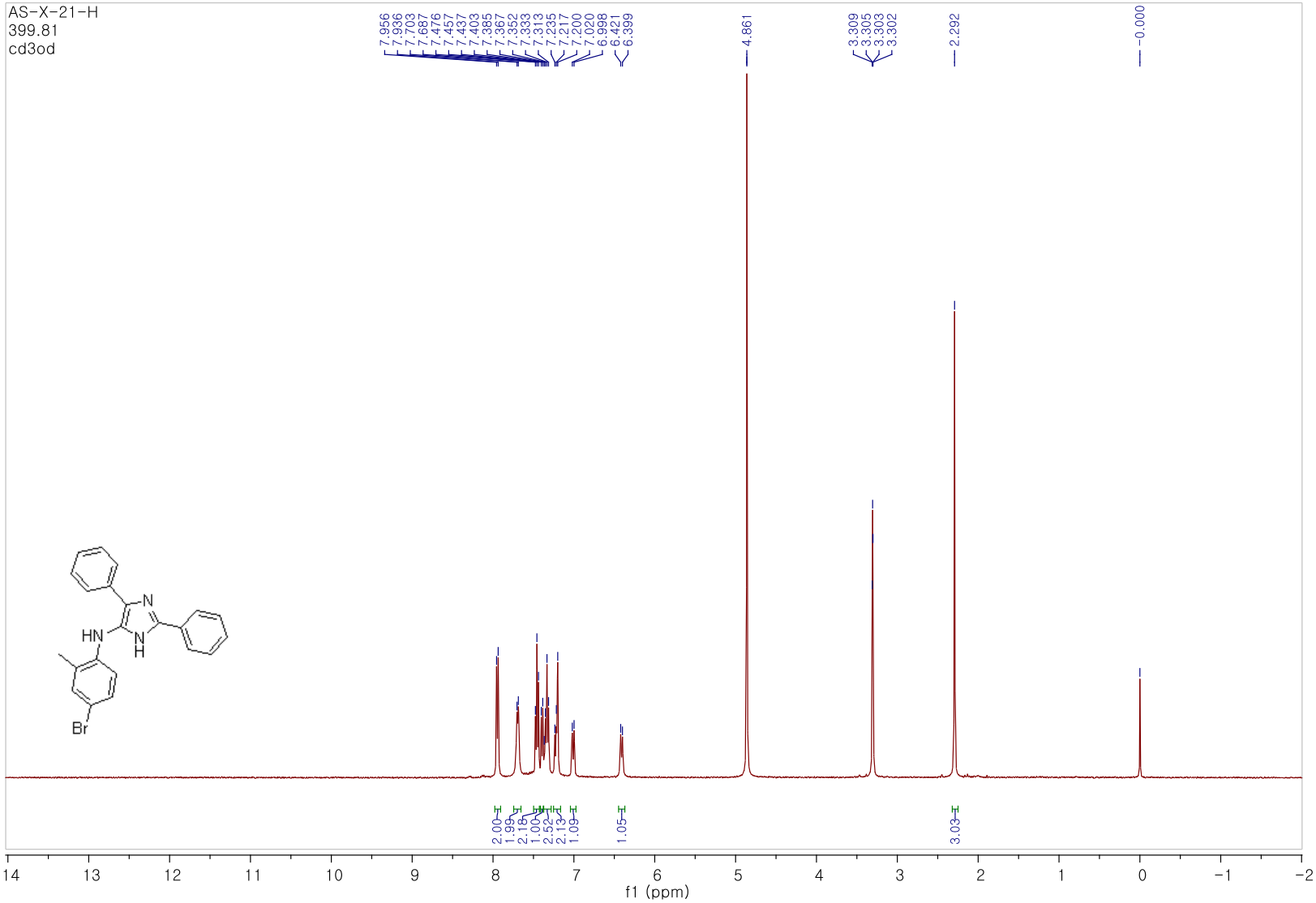
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4j**



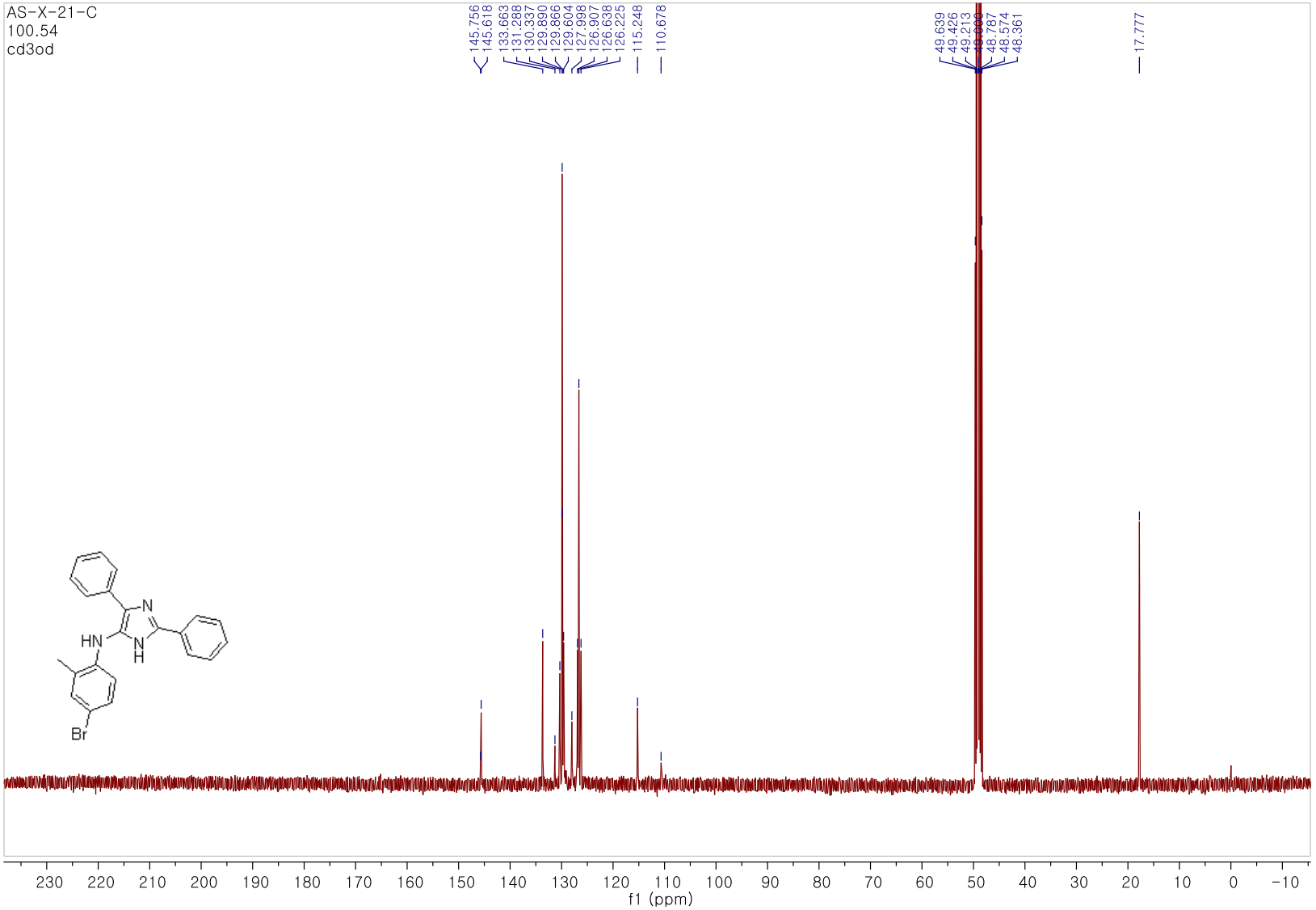
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4j**



^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4k**

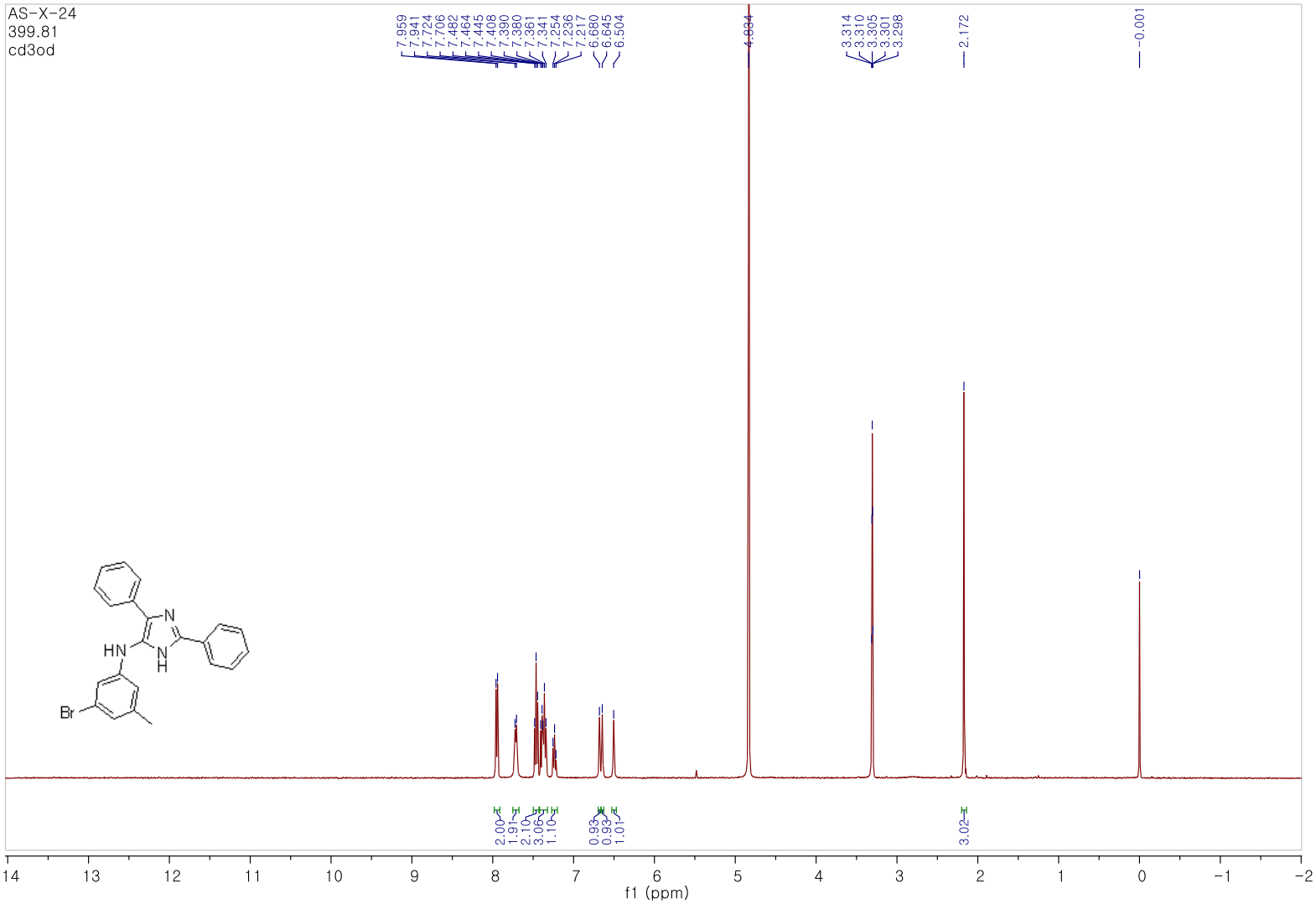


^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4k**

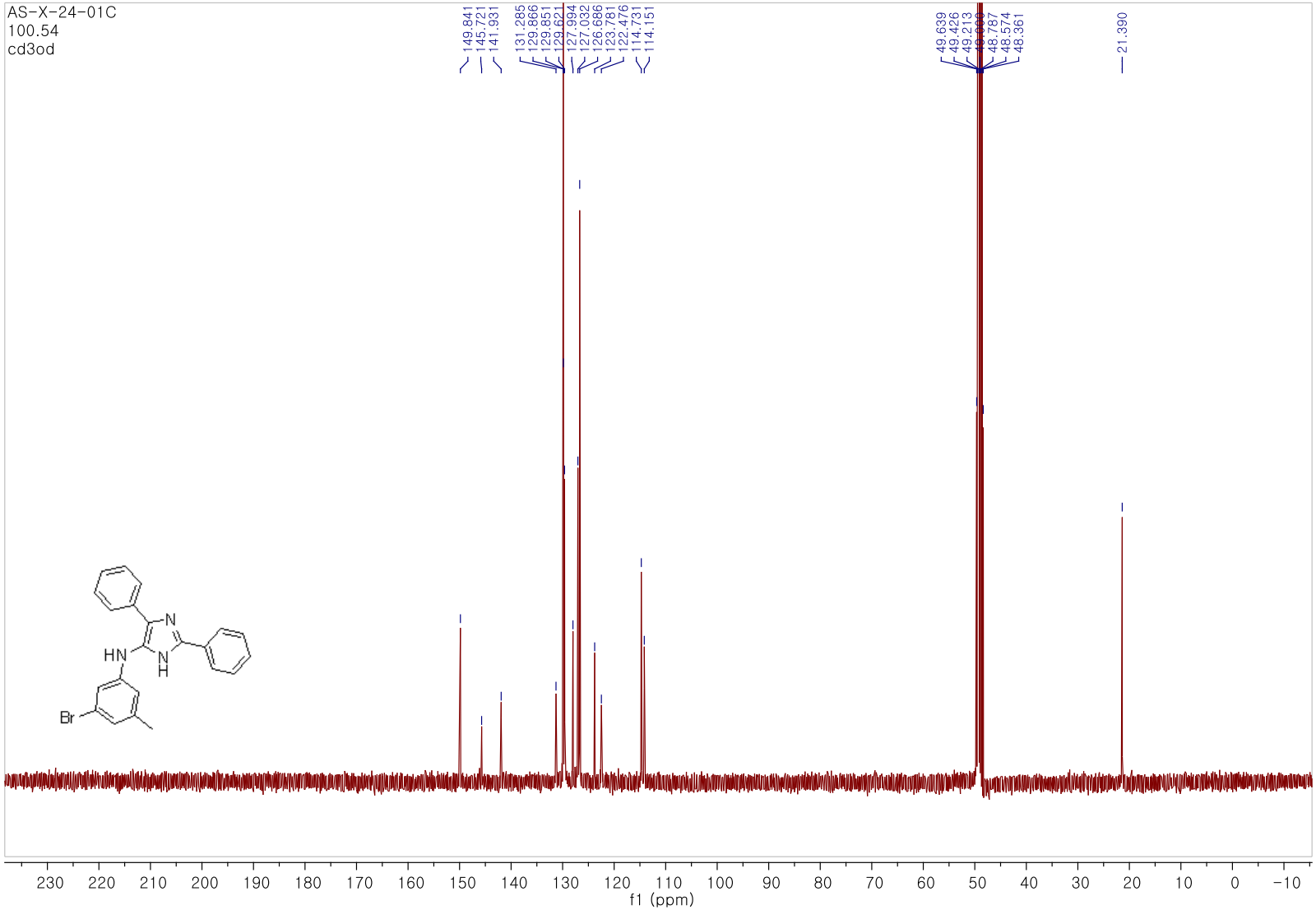


^{1}H NMR (400

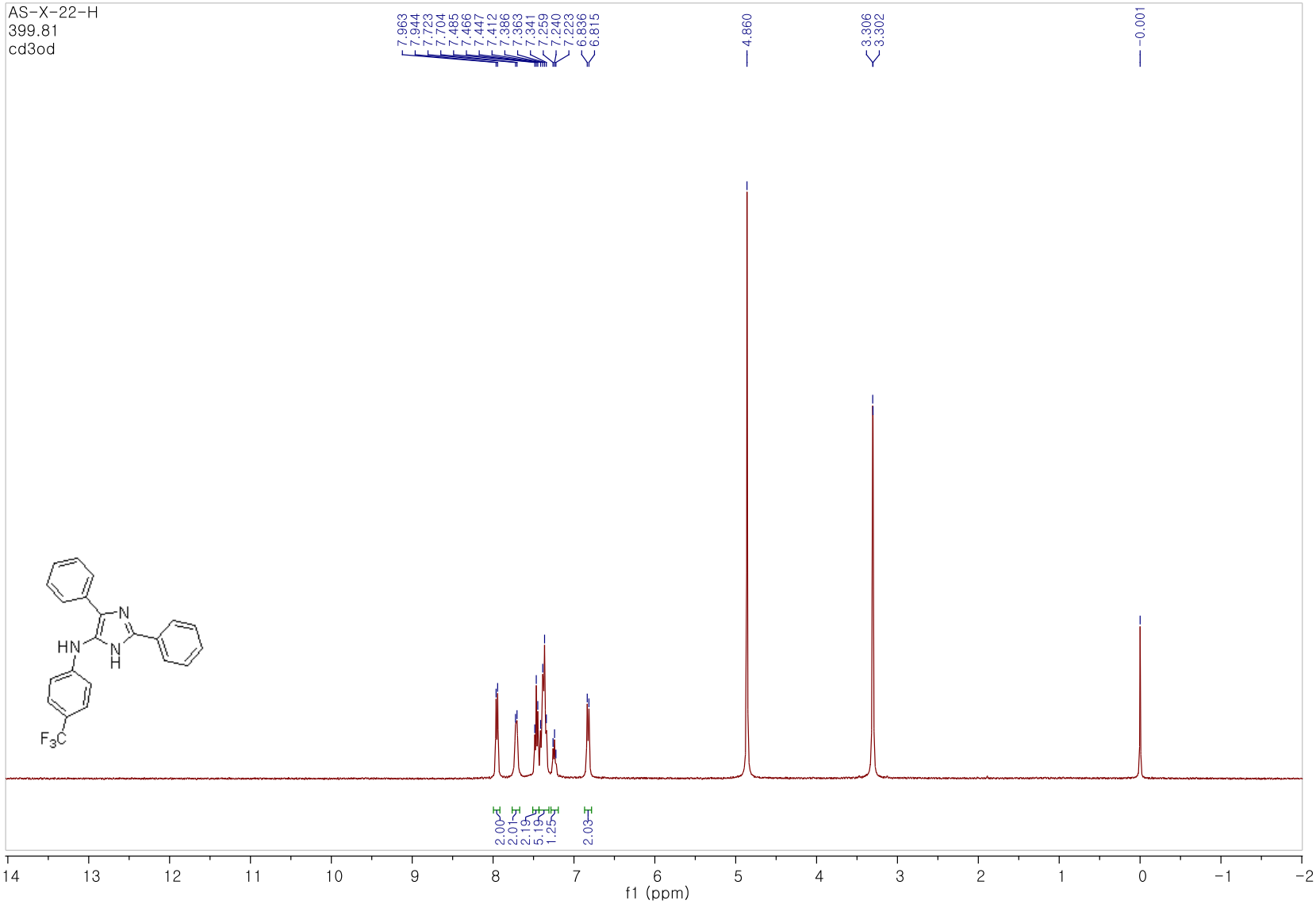
MHz, methanol-d_4) spectrum of **4l**



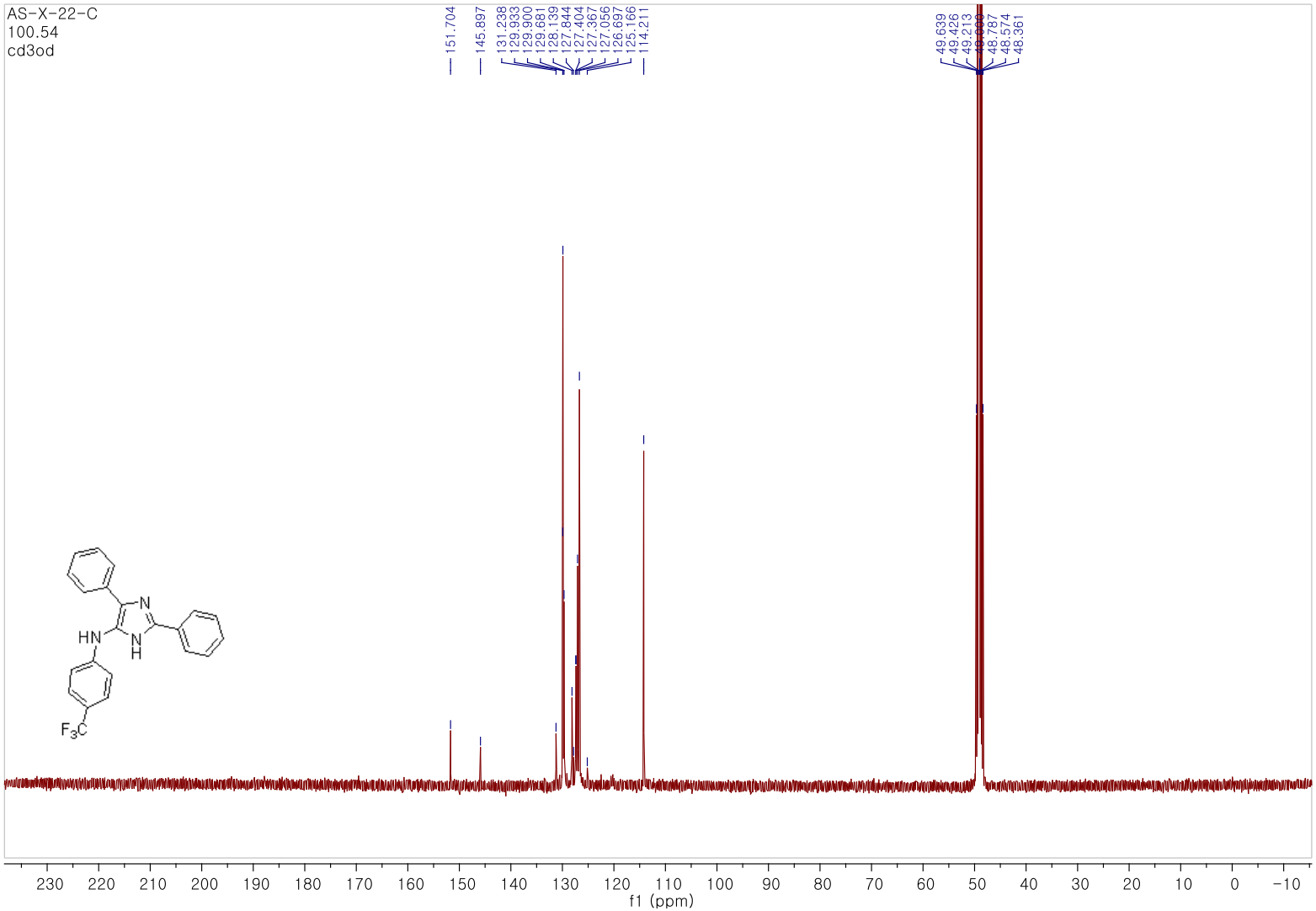
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4l**



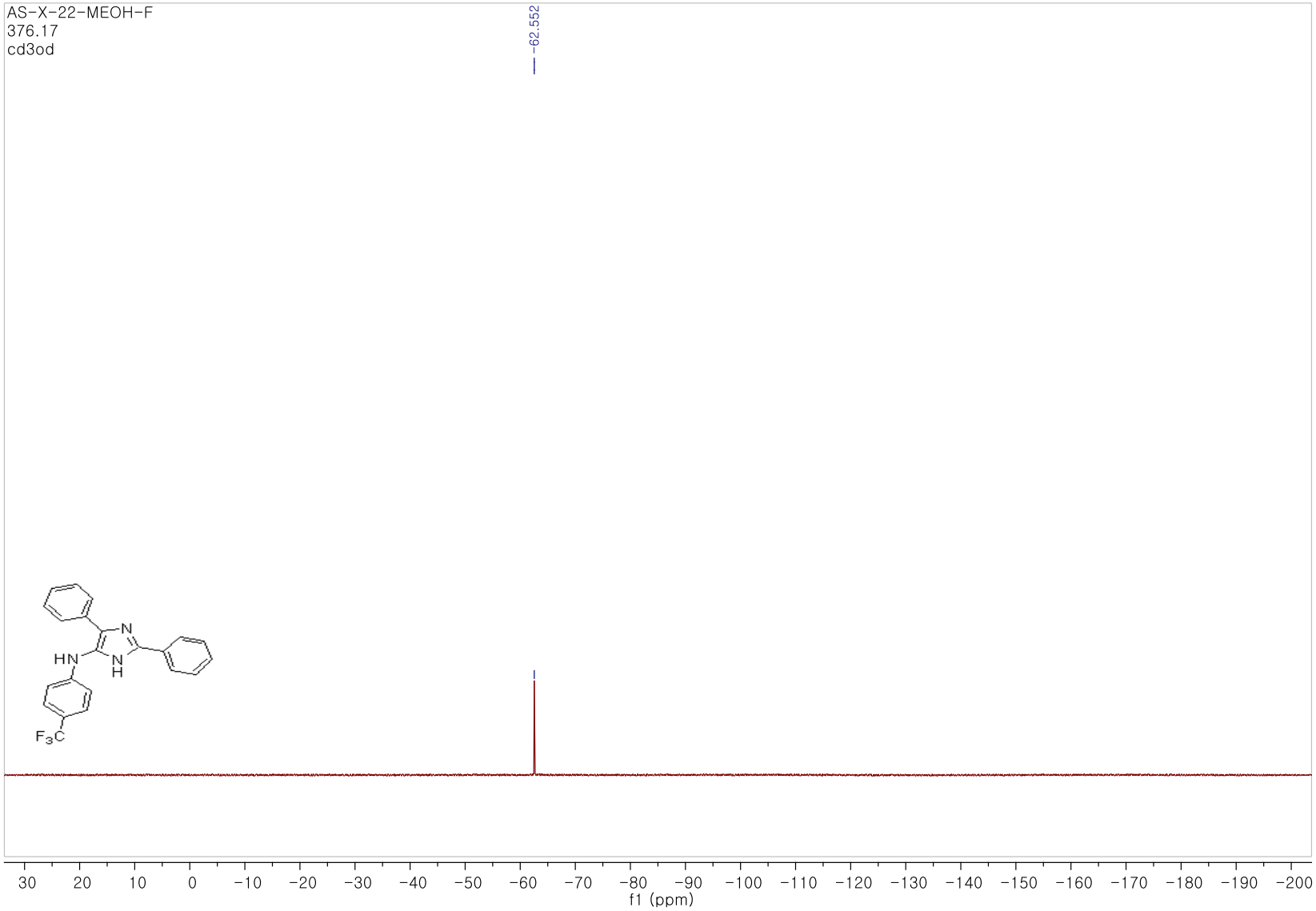
^{1}H NMR (400 MHz, methanol-*d*$_4$) spectrum of **4m**



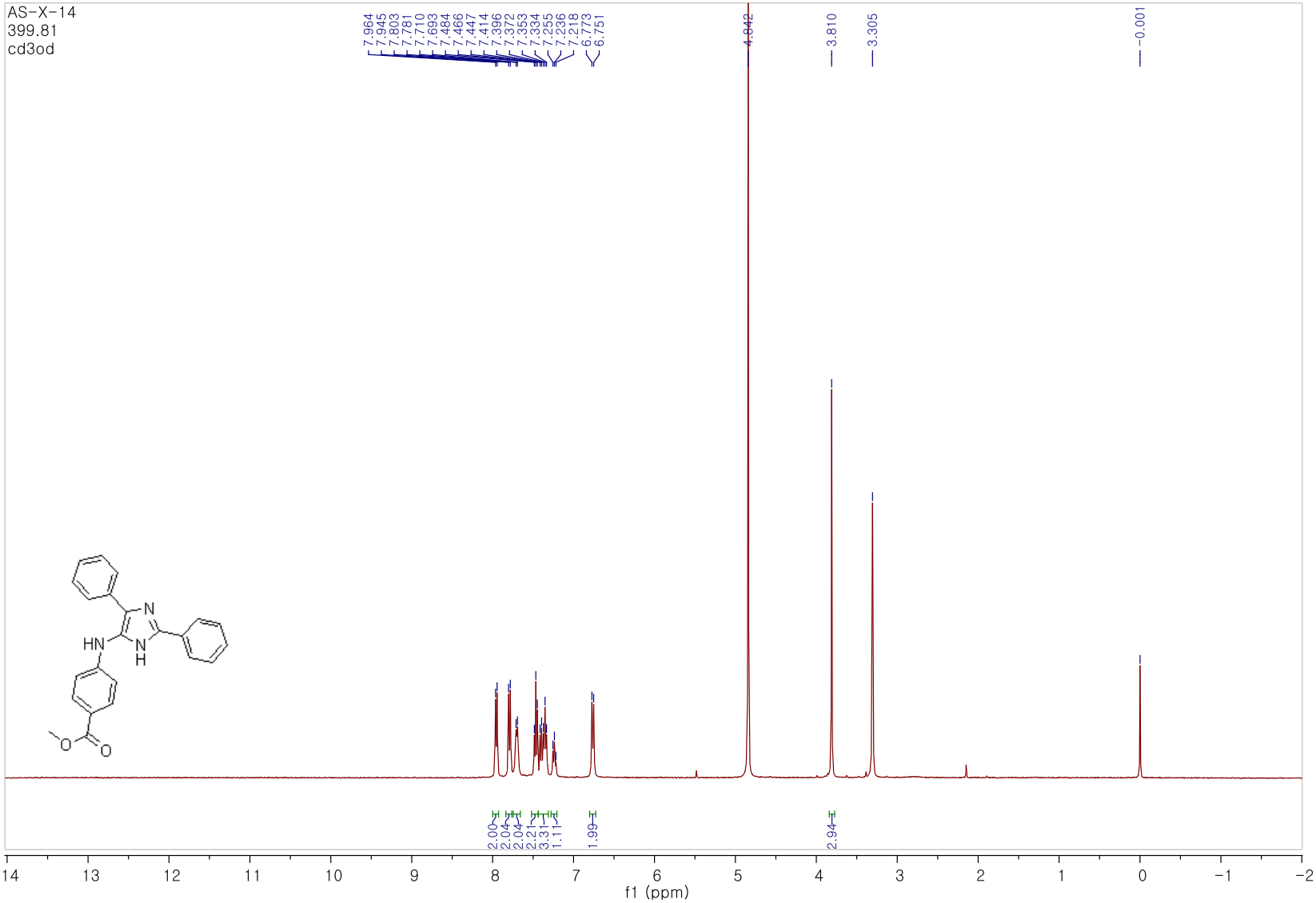
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4m**



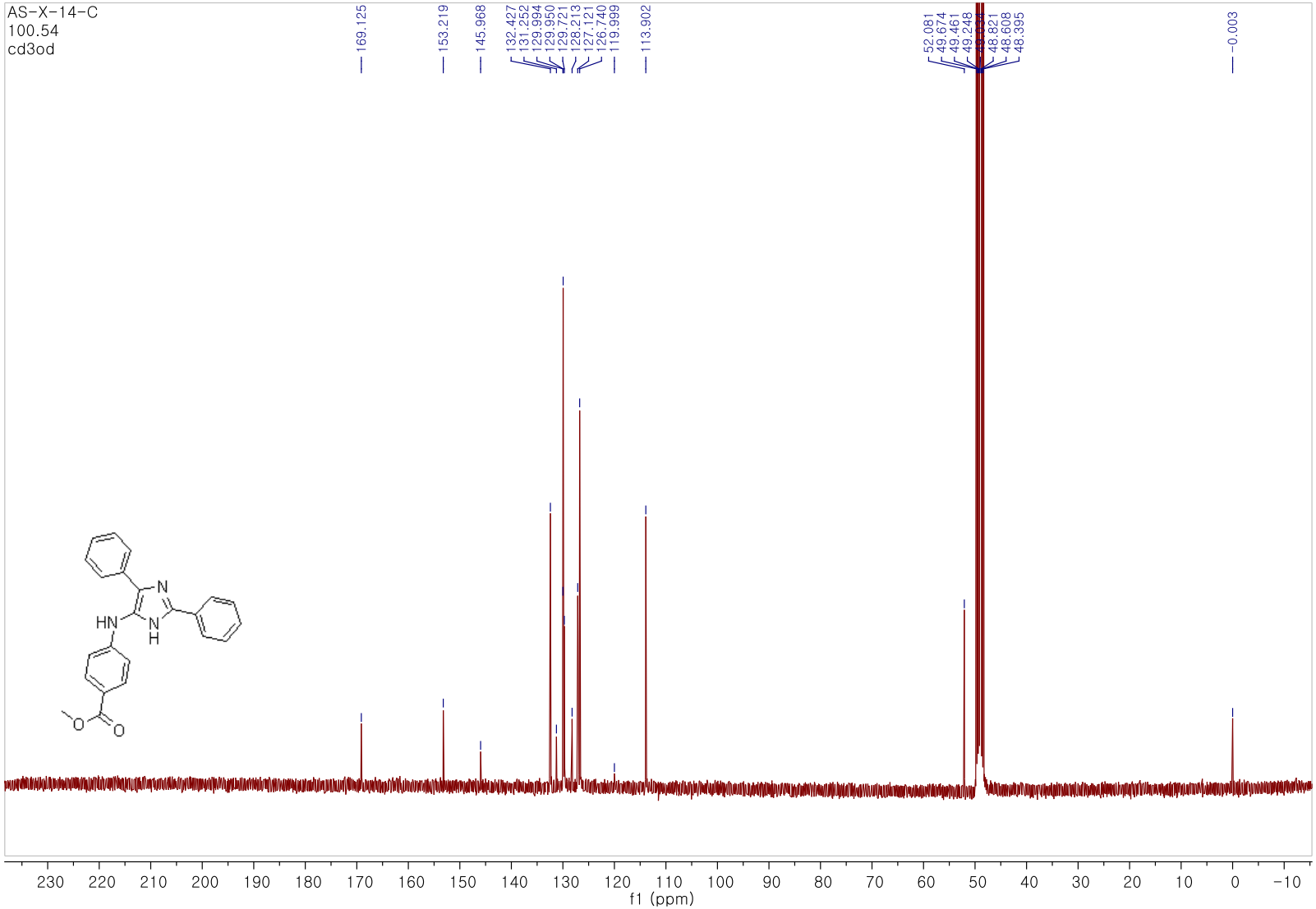
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4m**



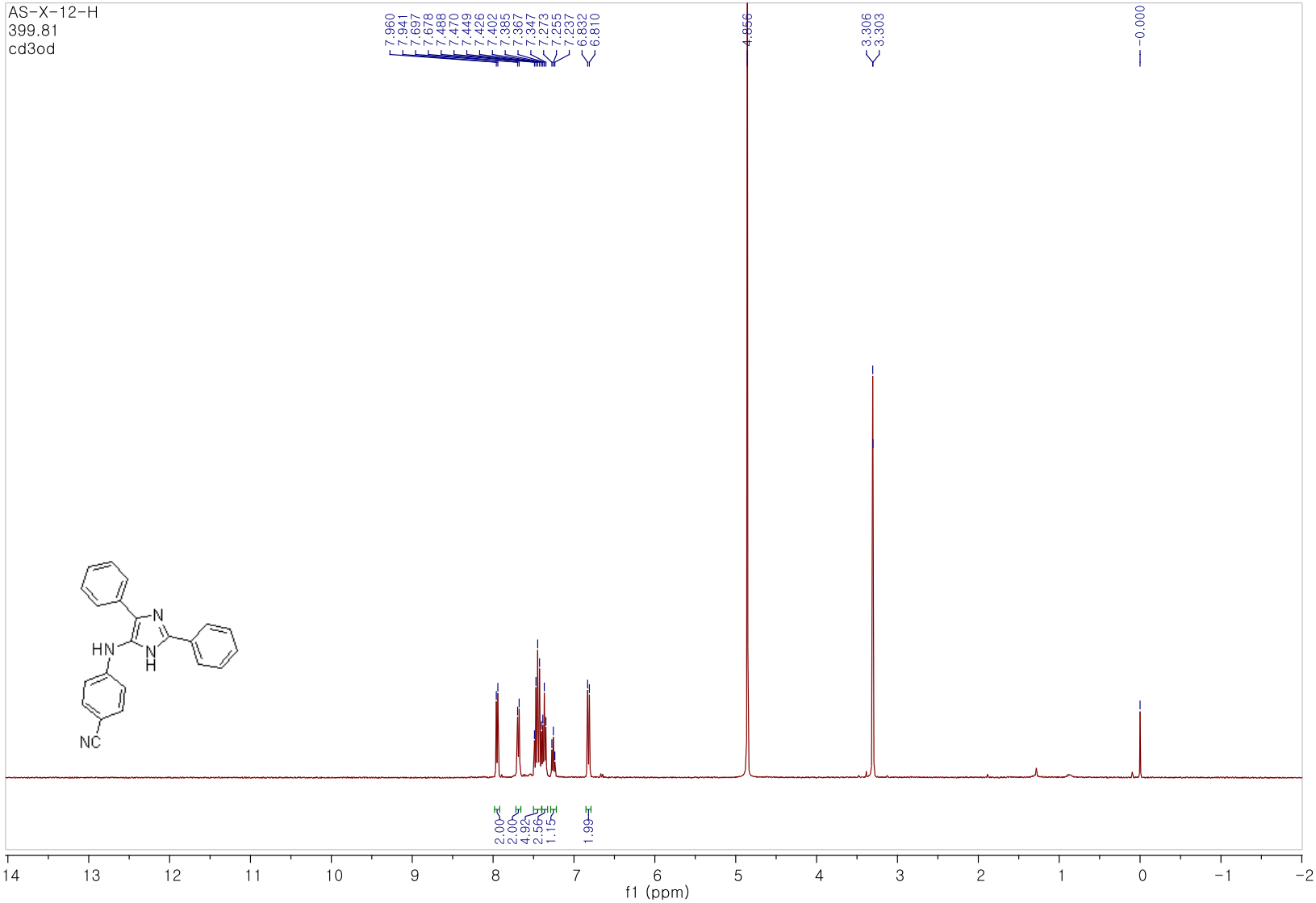
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4n**



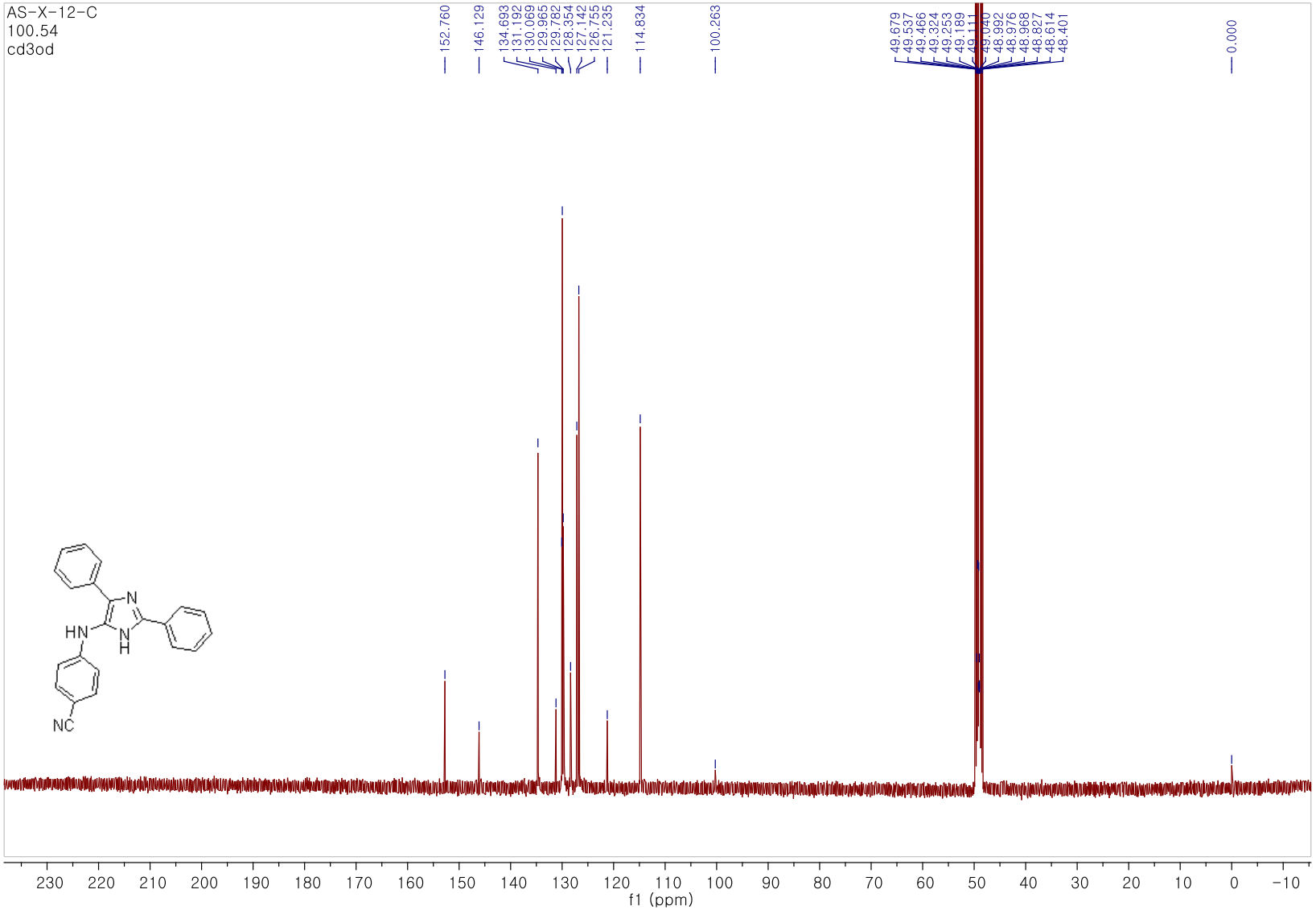
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4n**



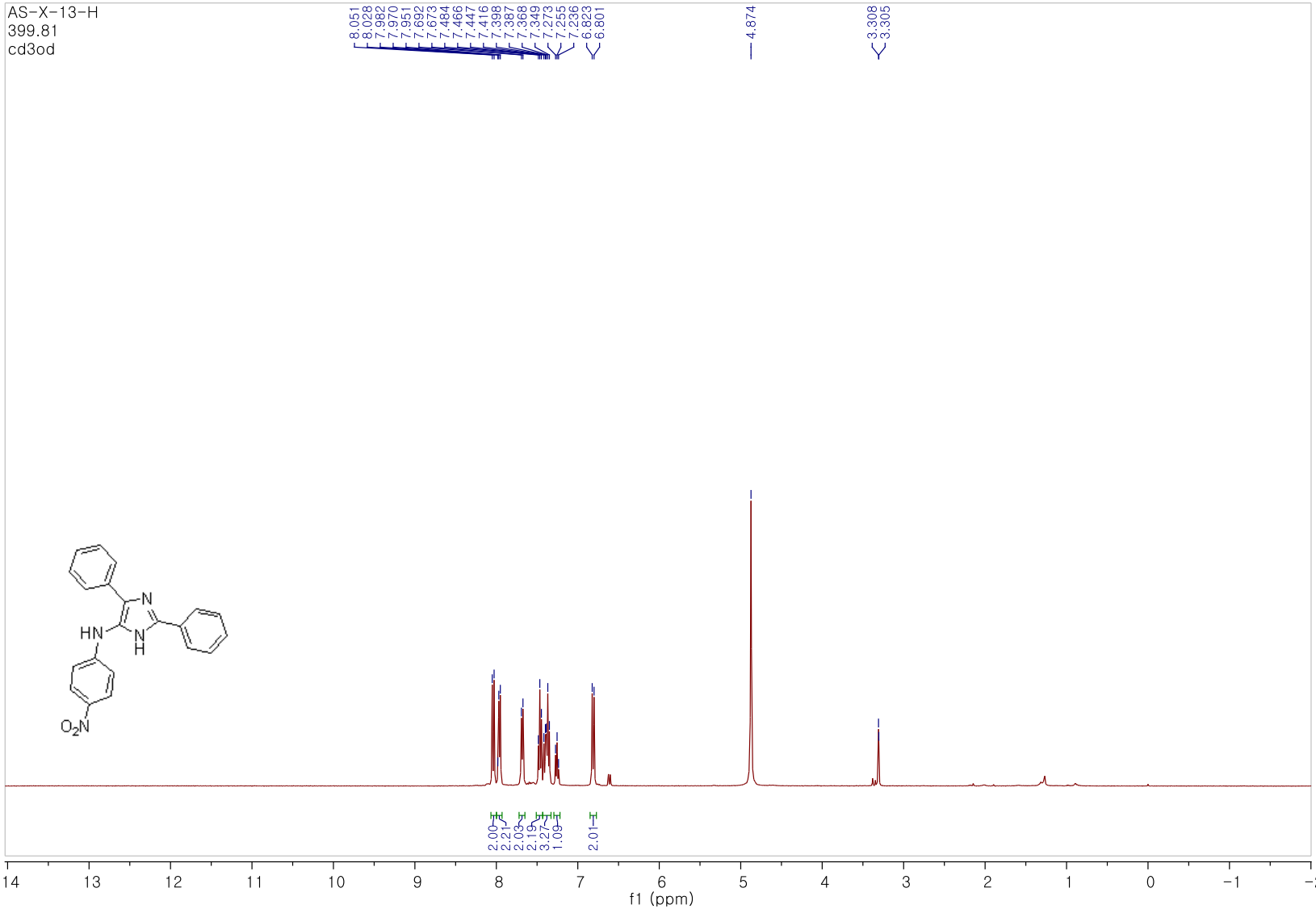
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4o**



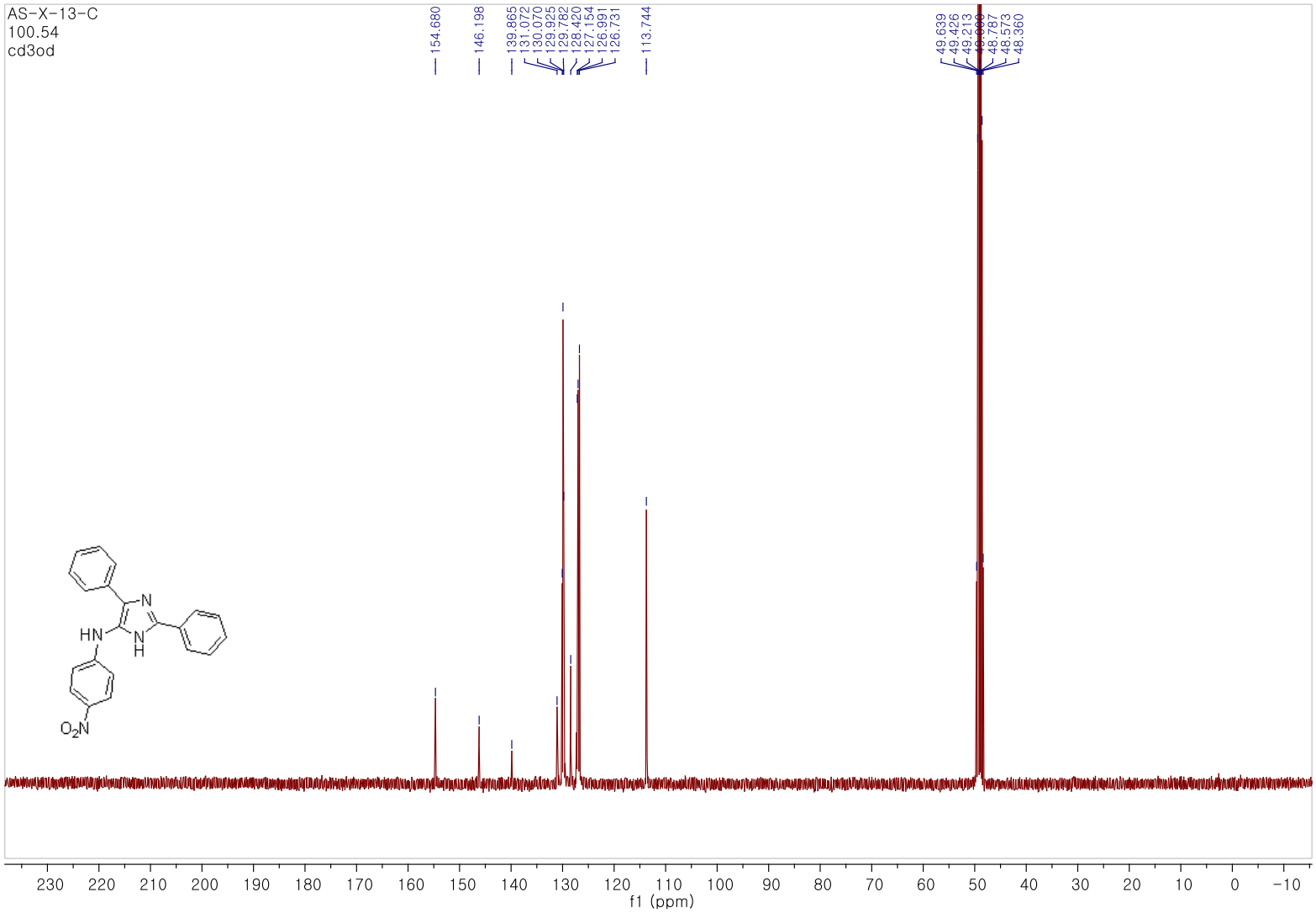
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4o**



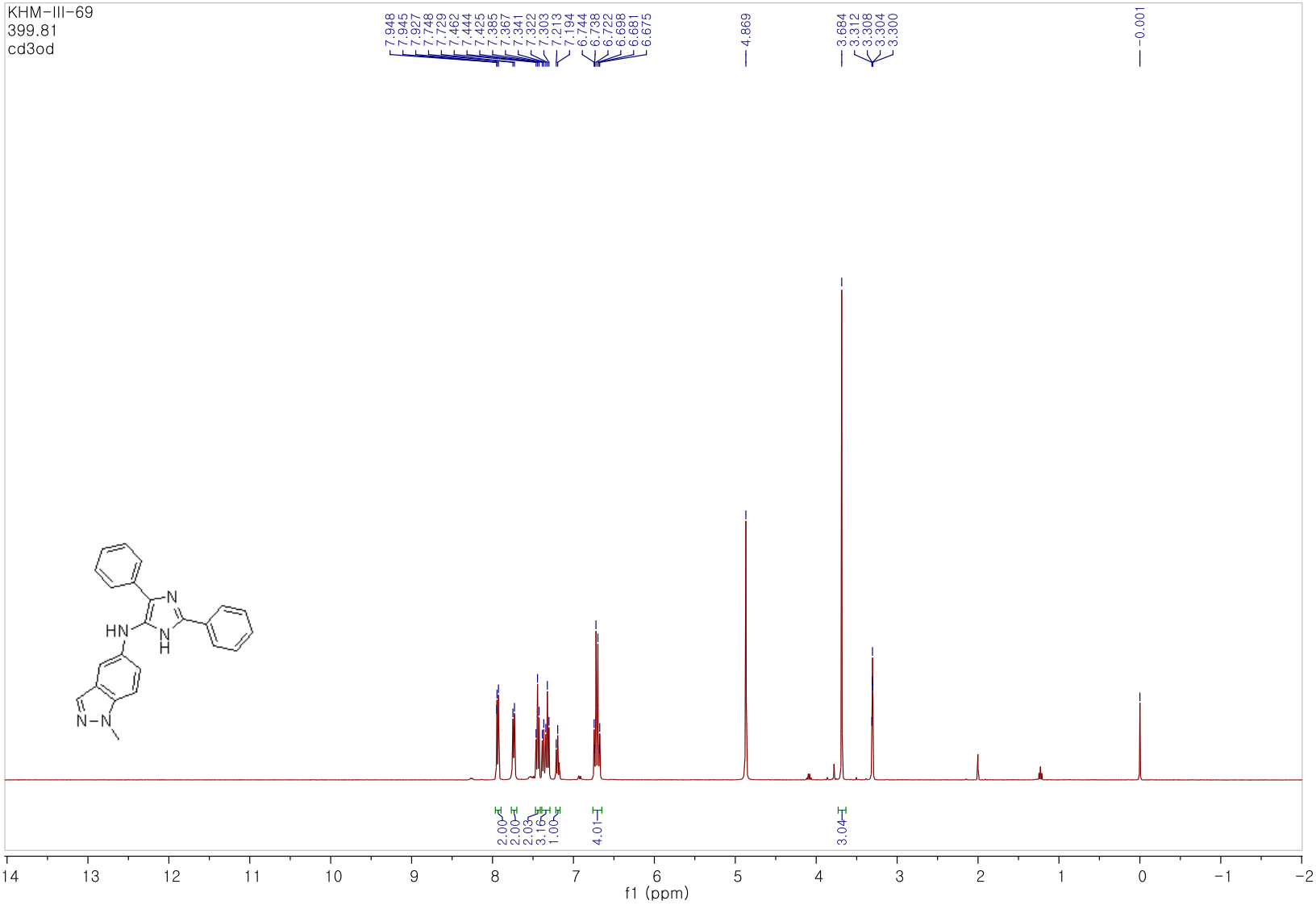
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4p**



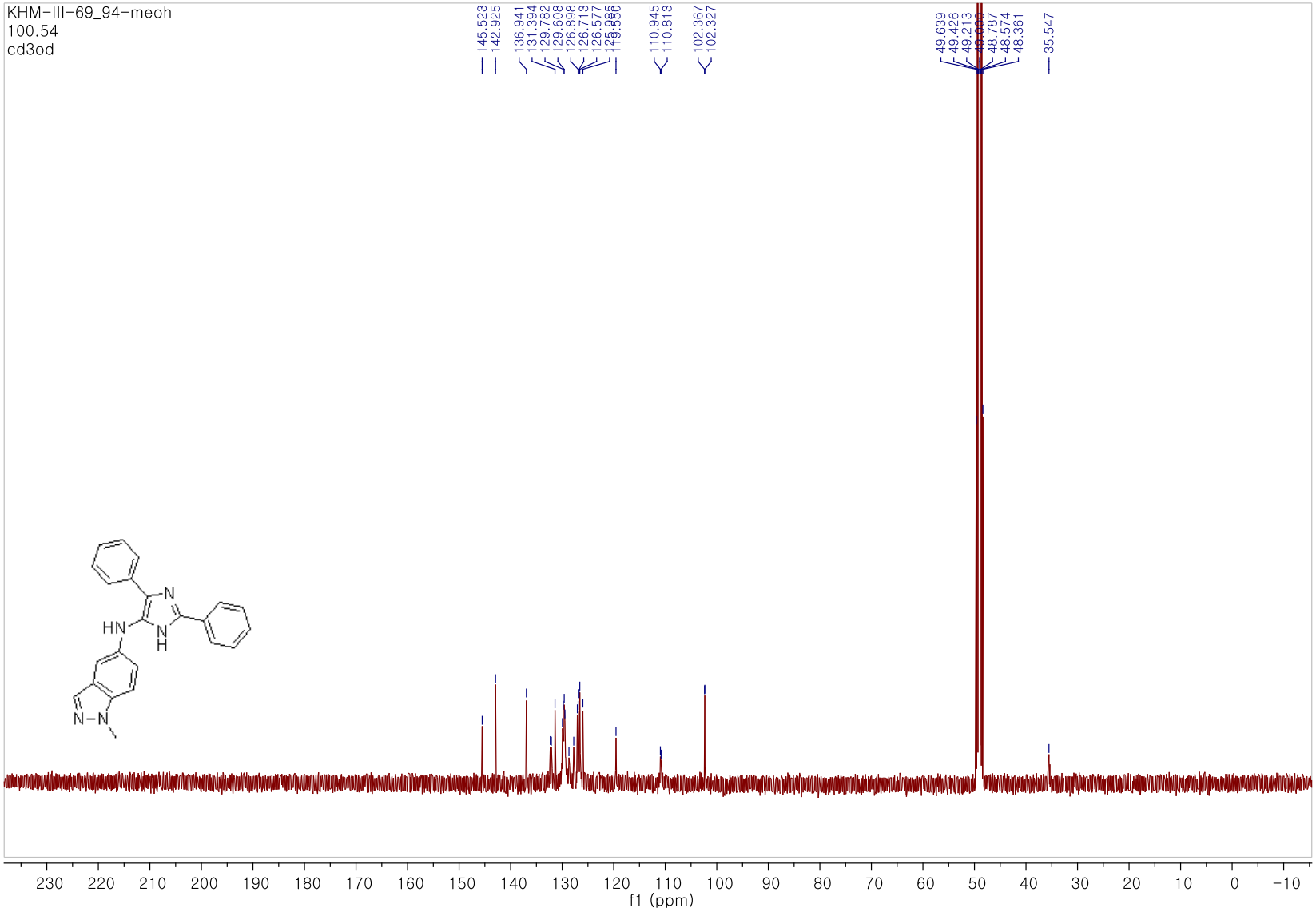
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4p**



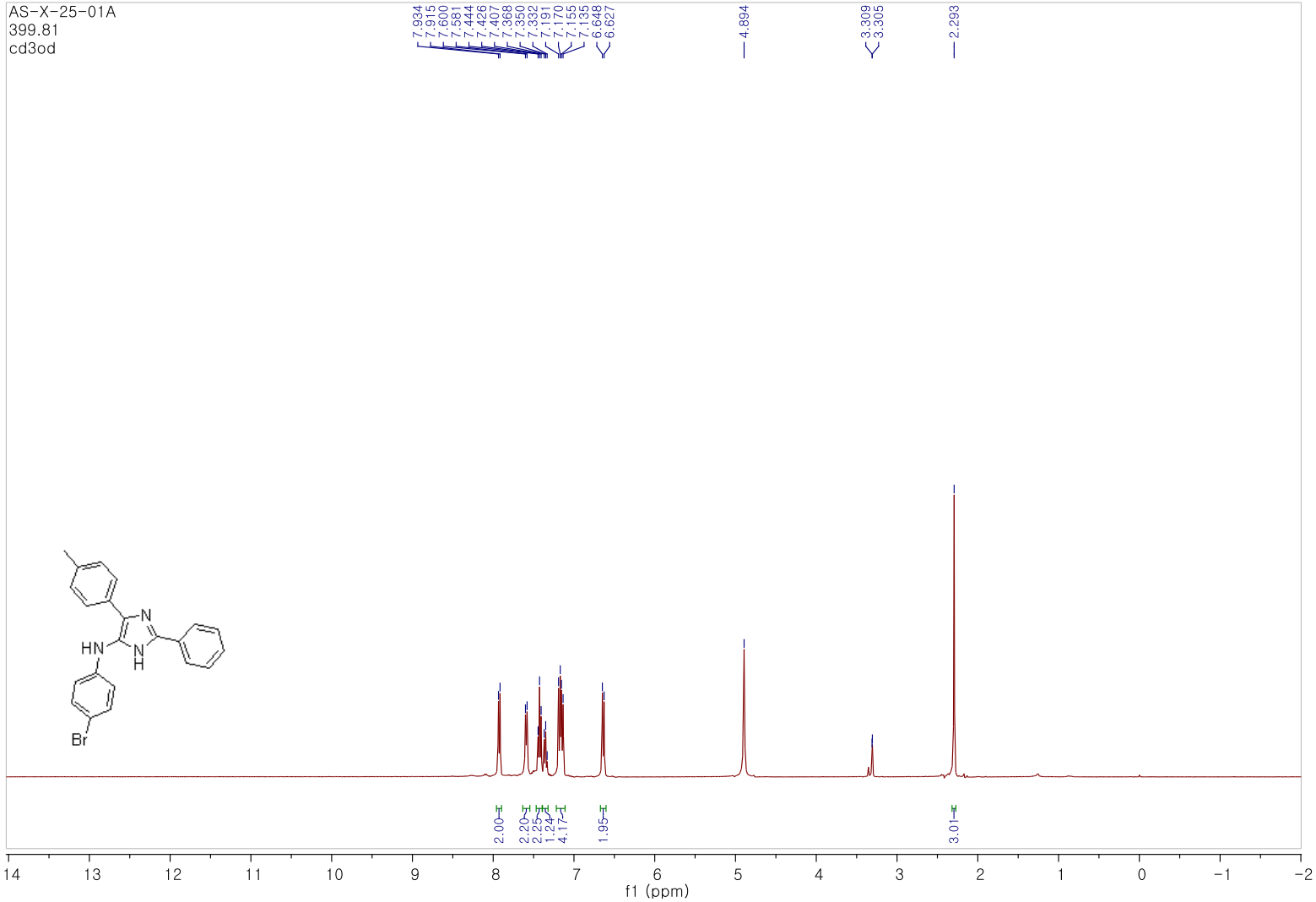
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4q**



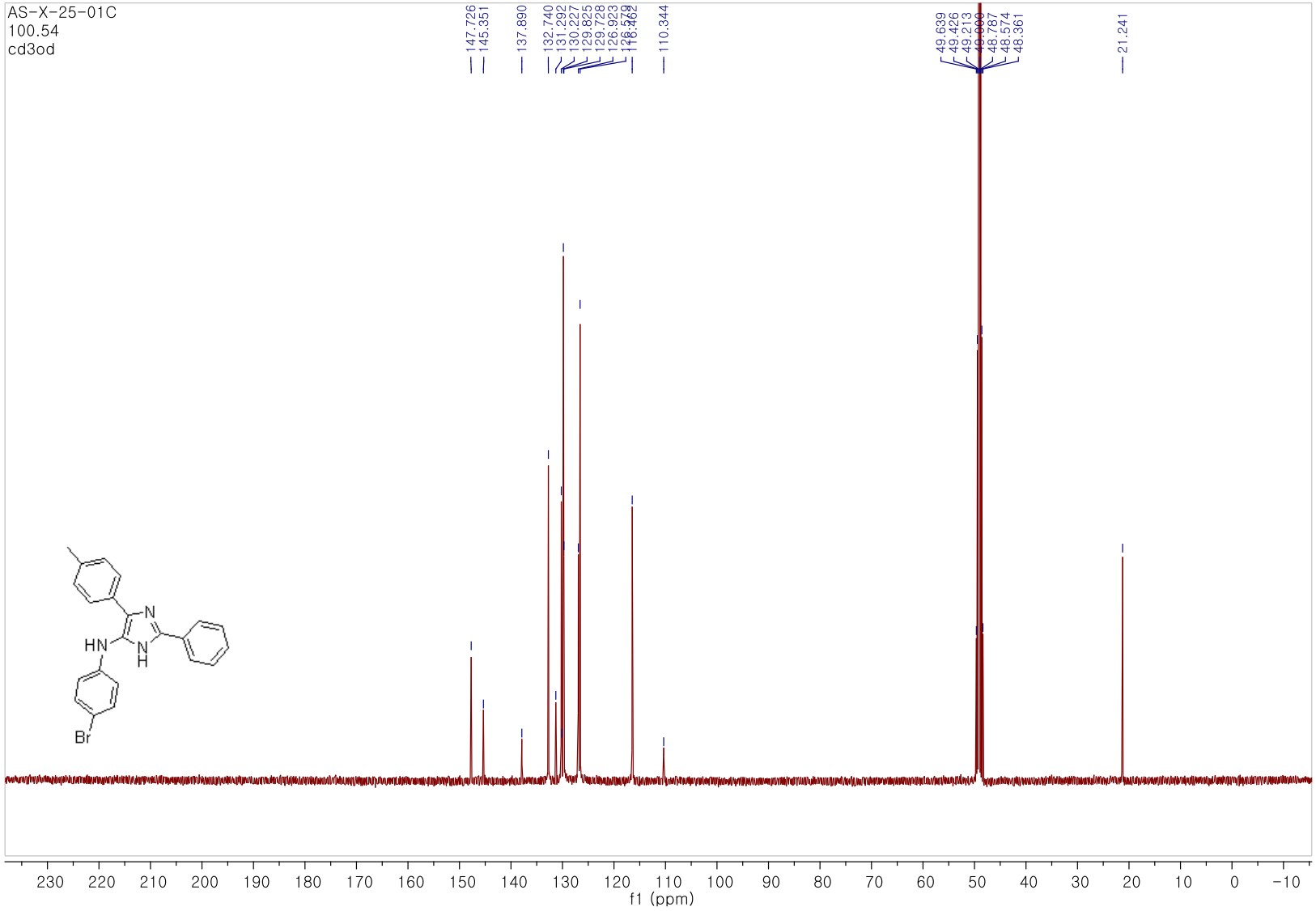
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4q**



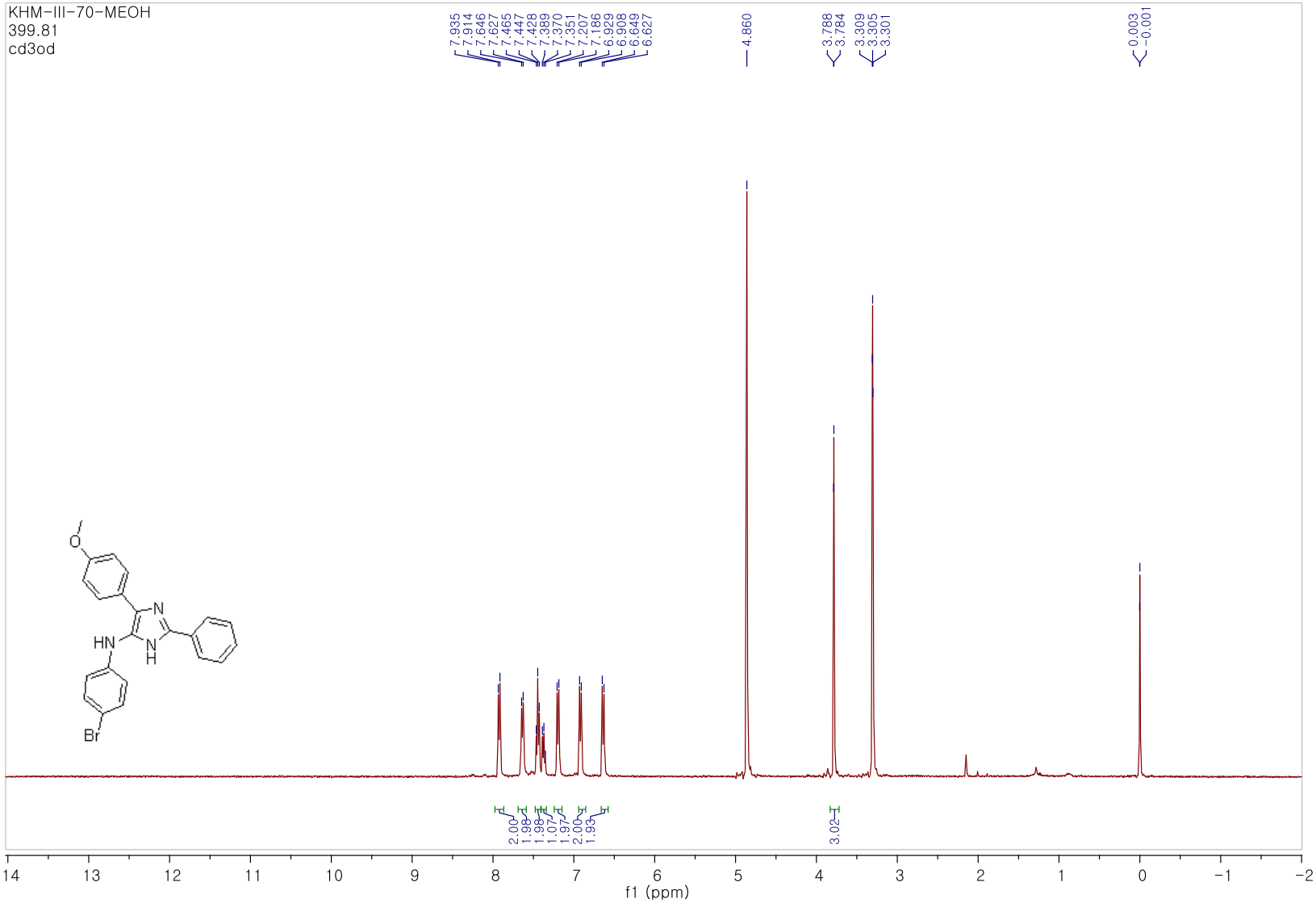
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4r**



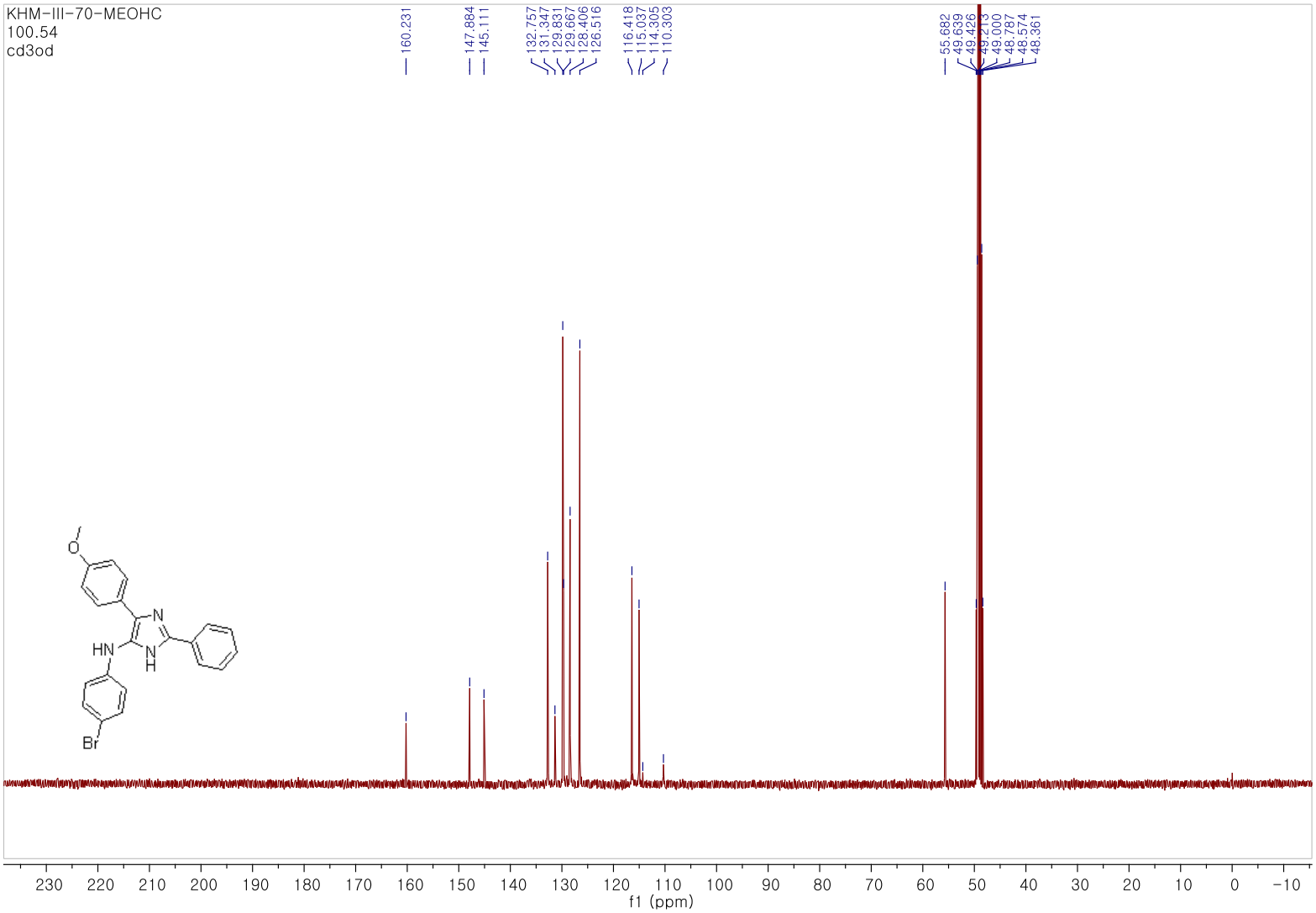
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4r**



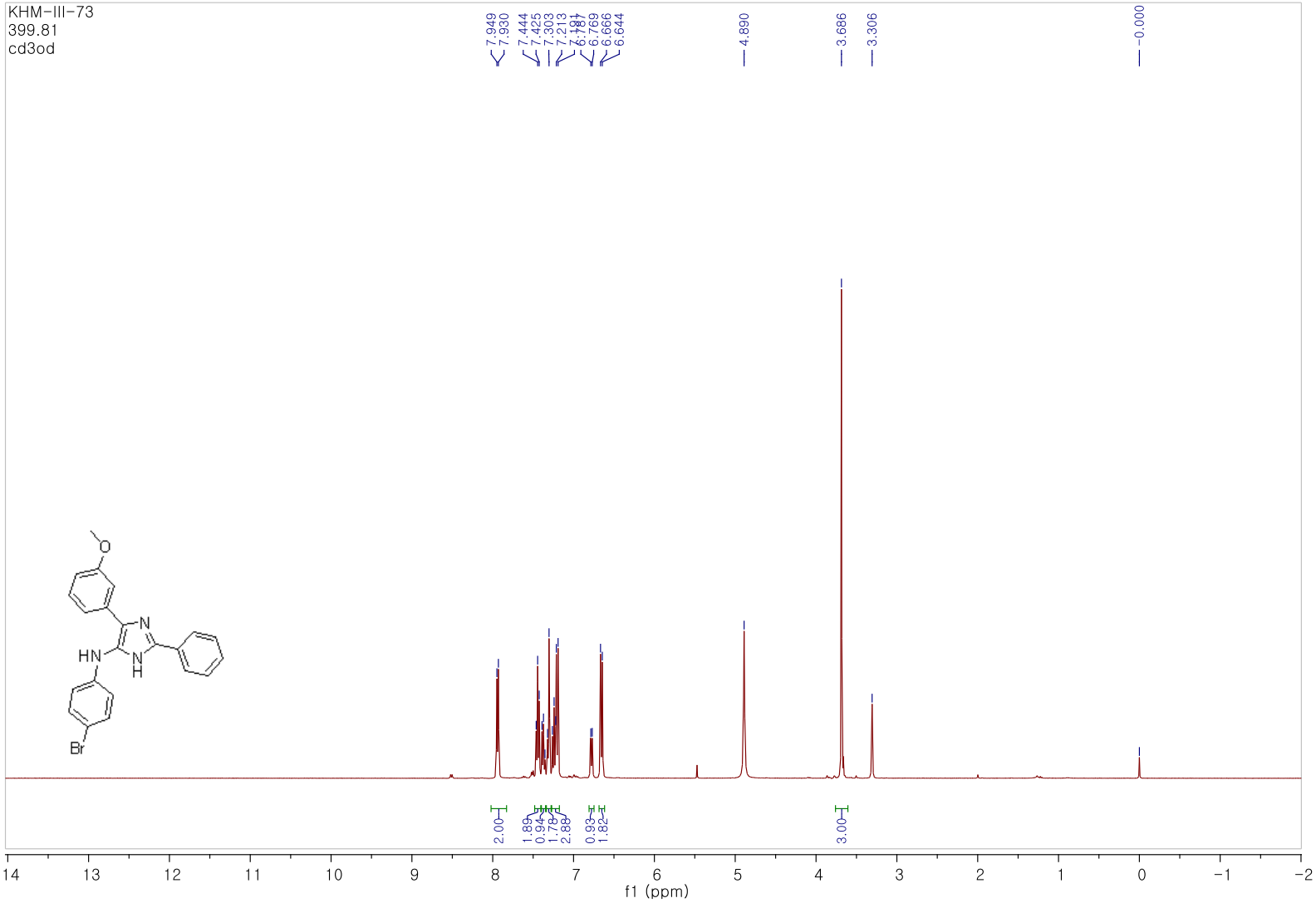
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4s**



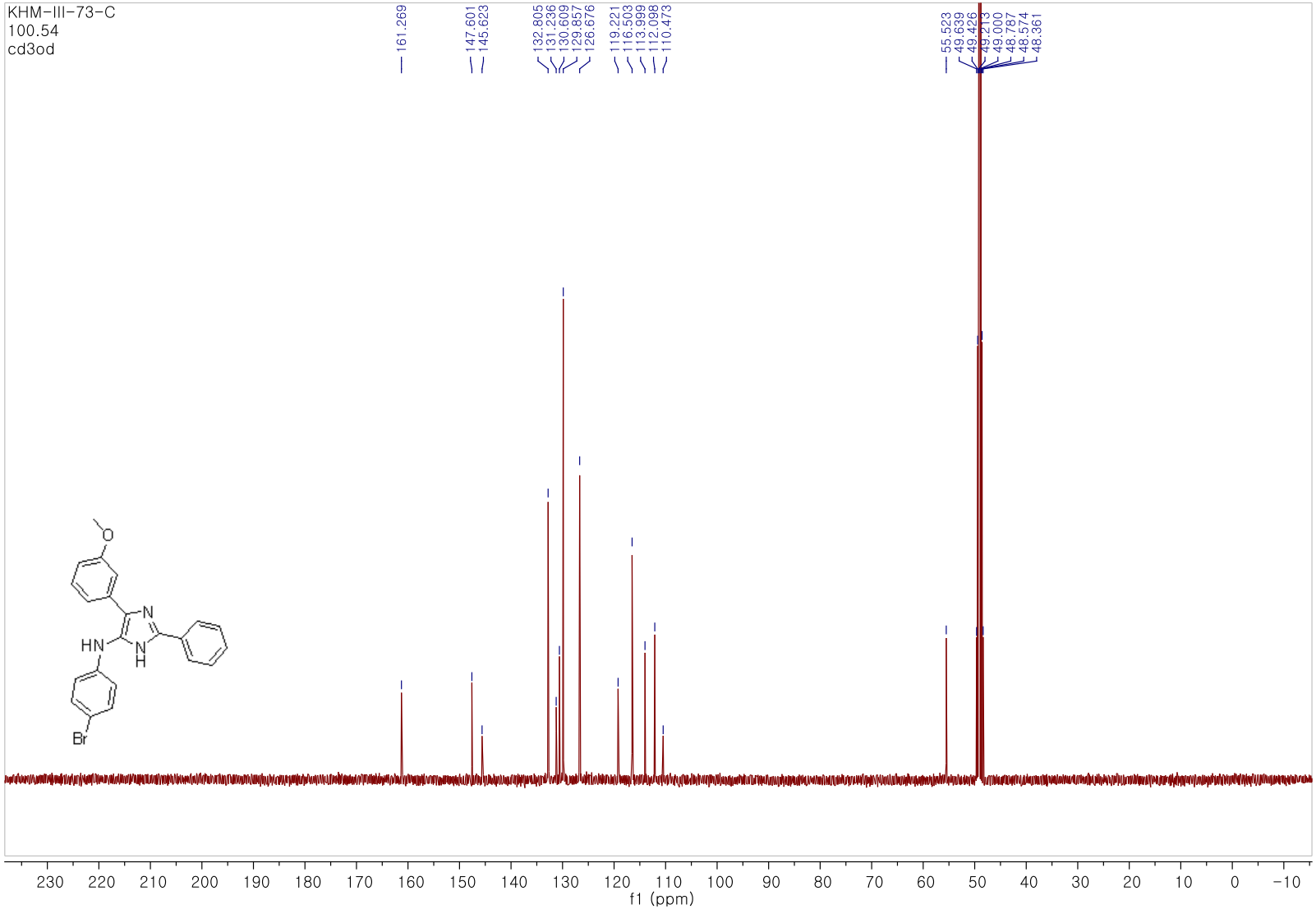
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4s**



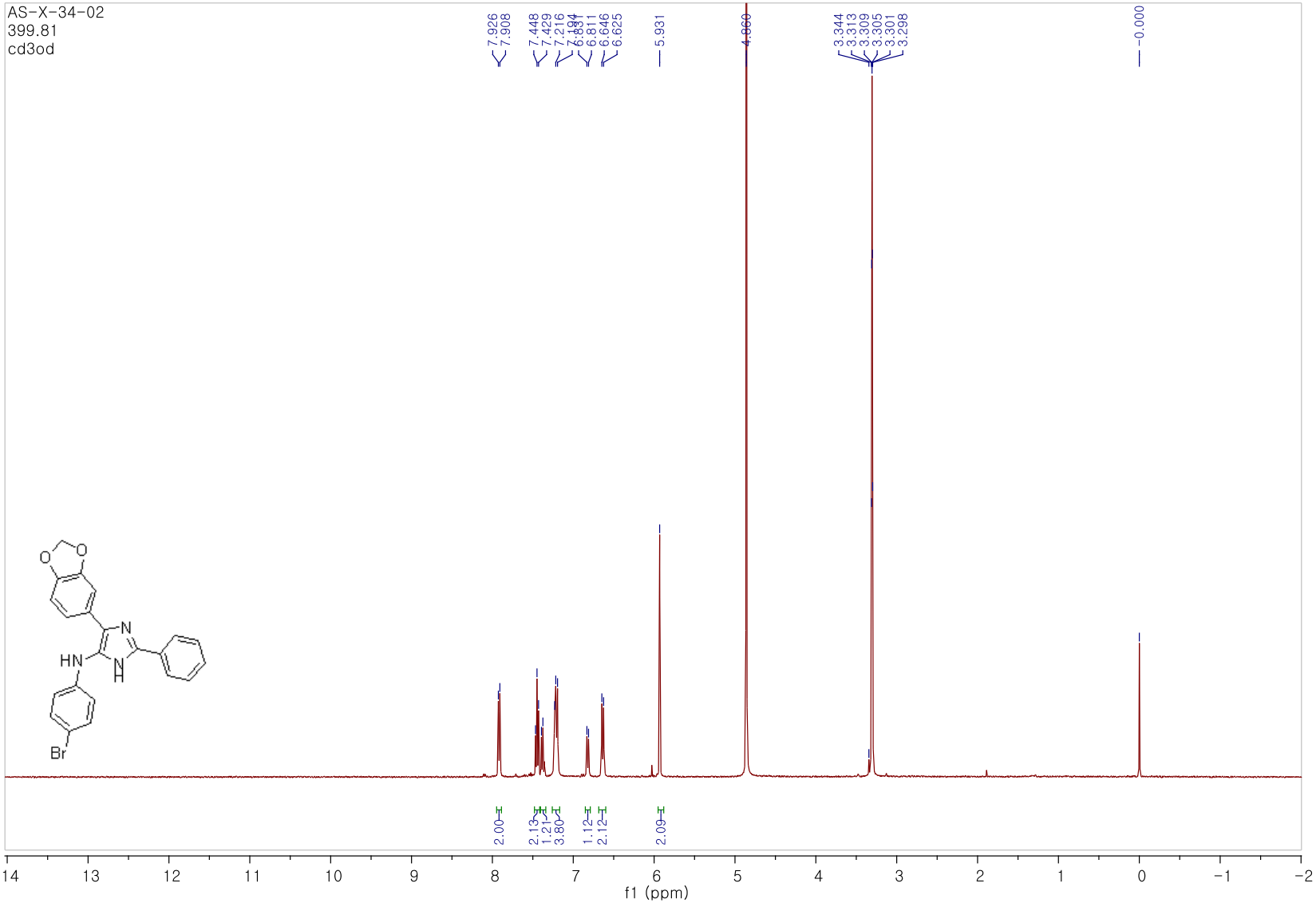
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4t**



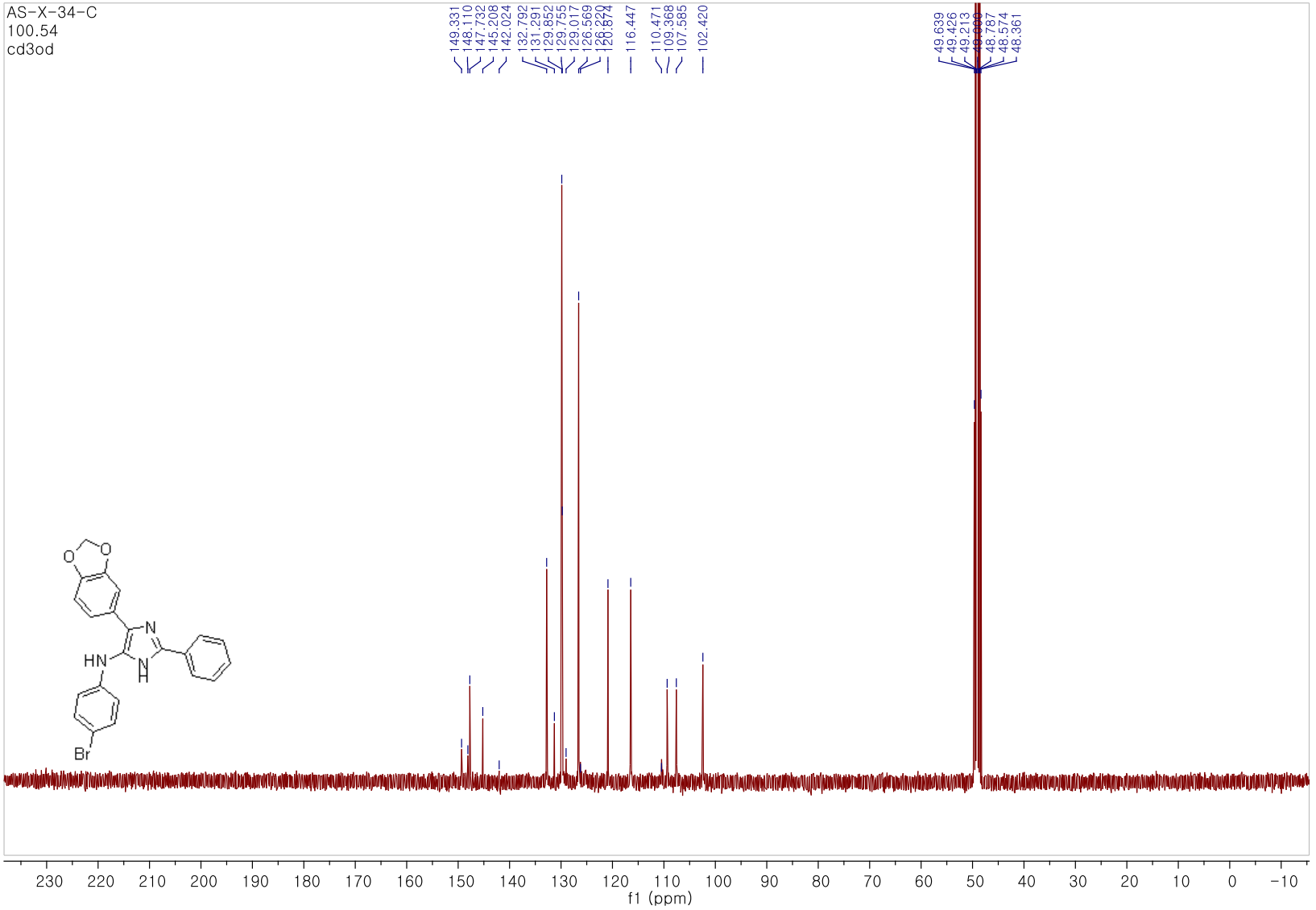
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4t**



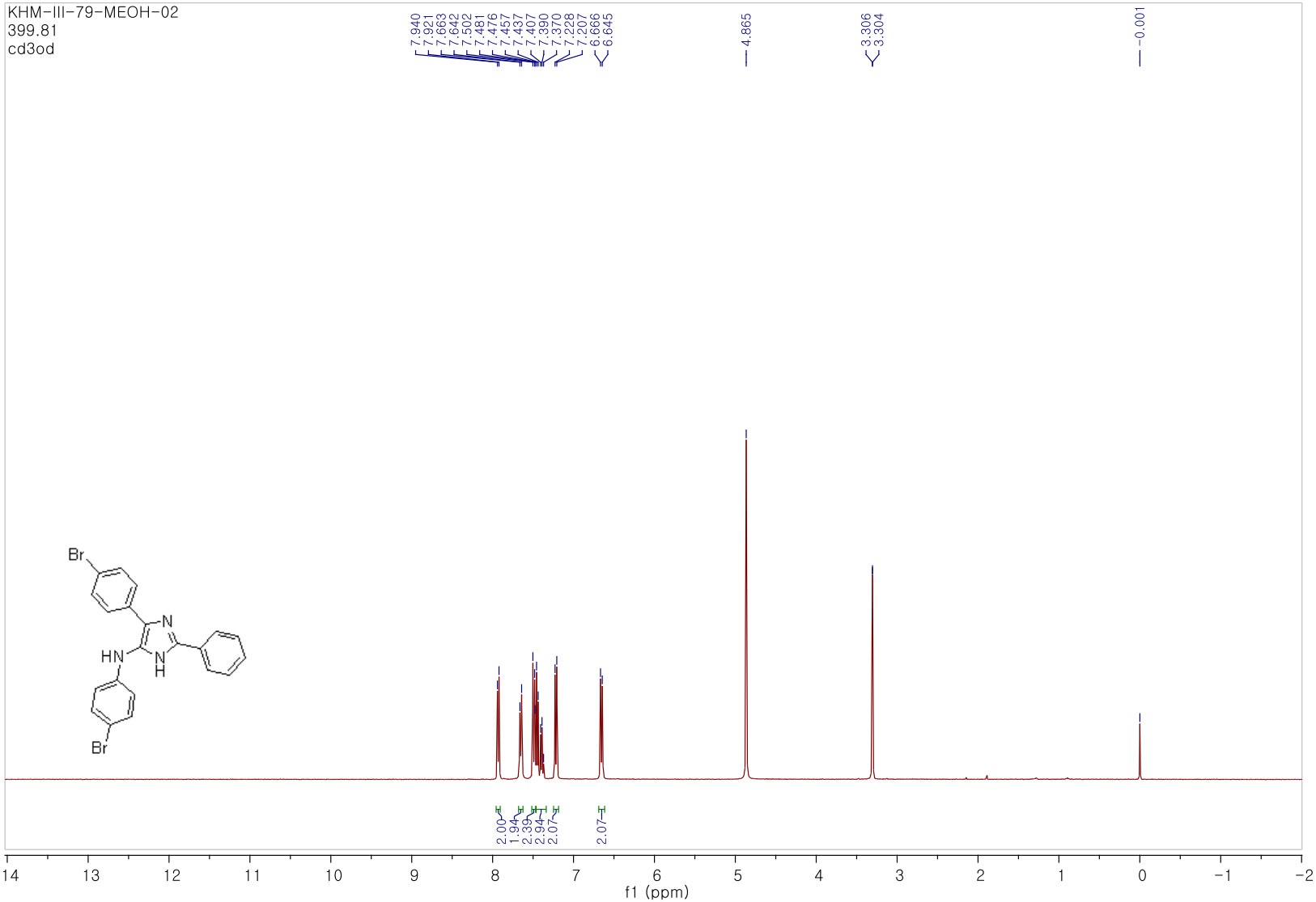
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4u**



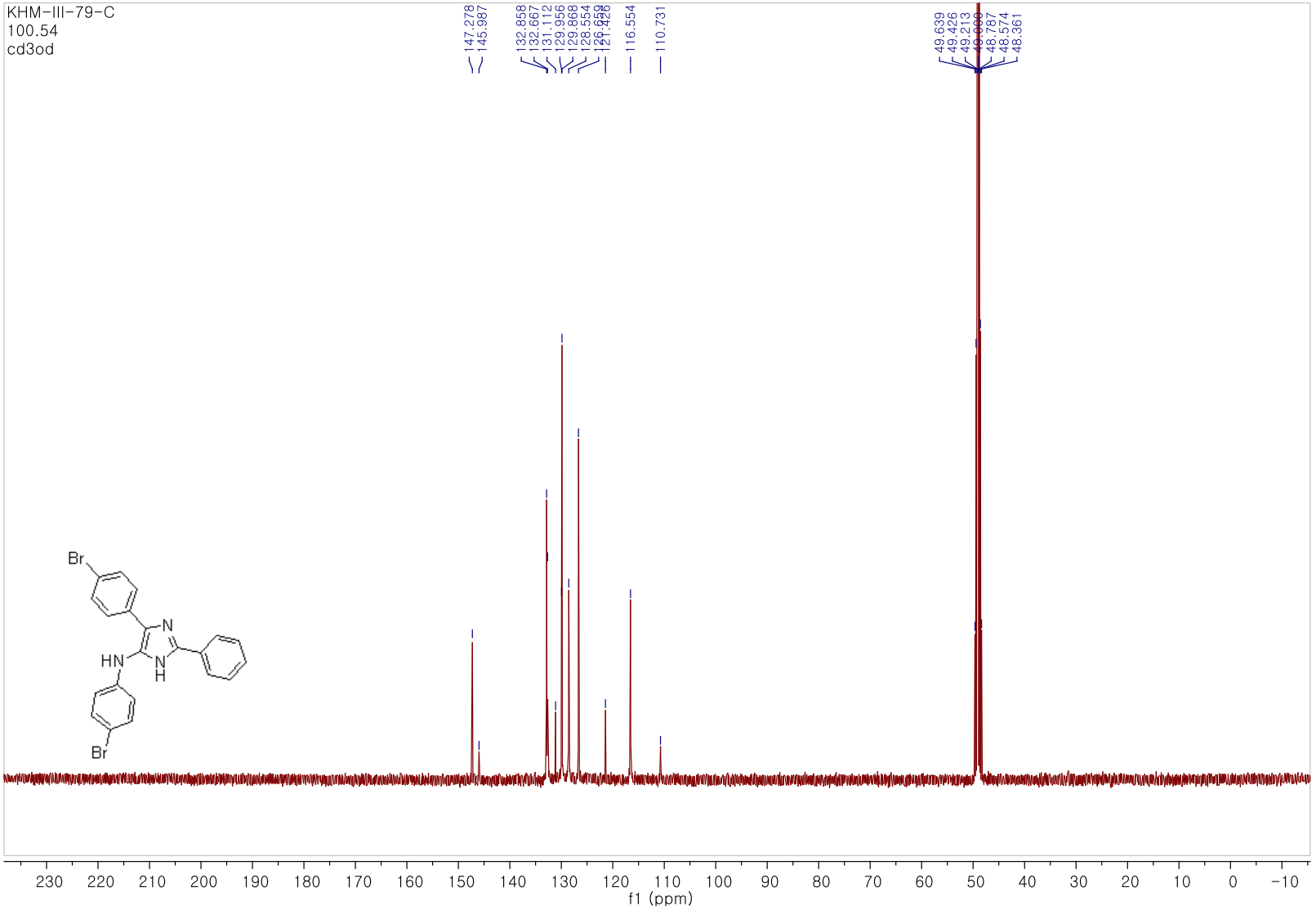
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4u**



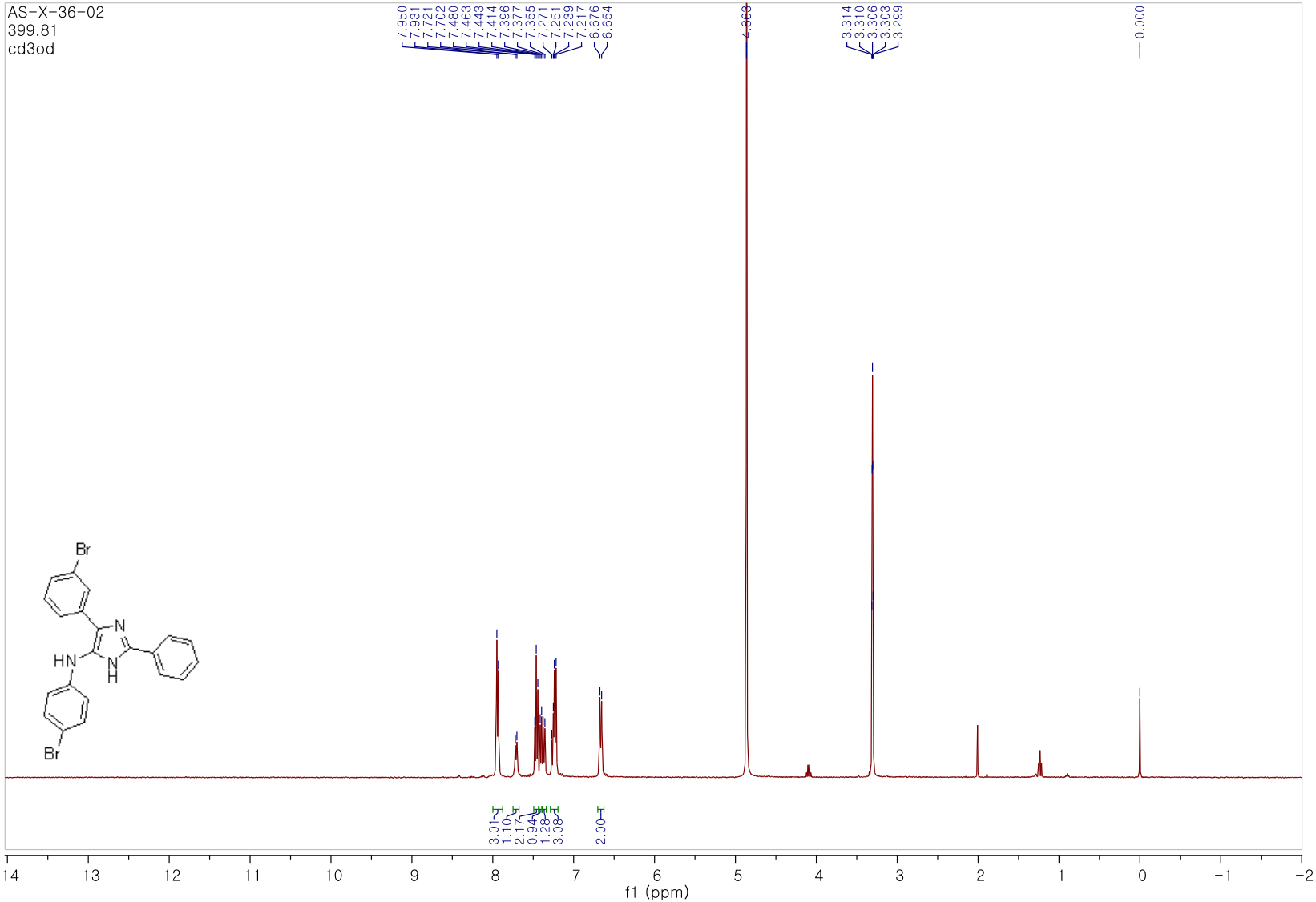
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4v**



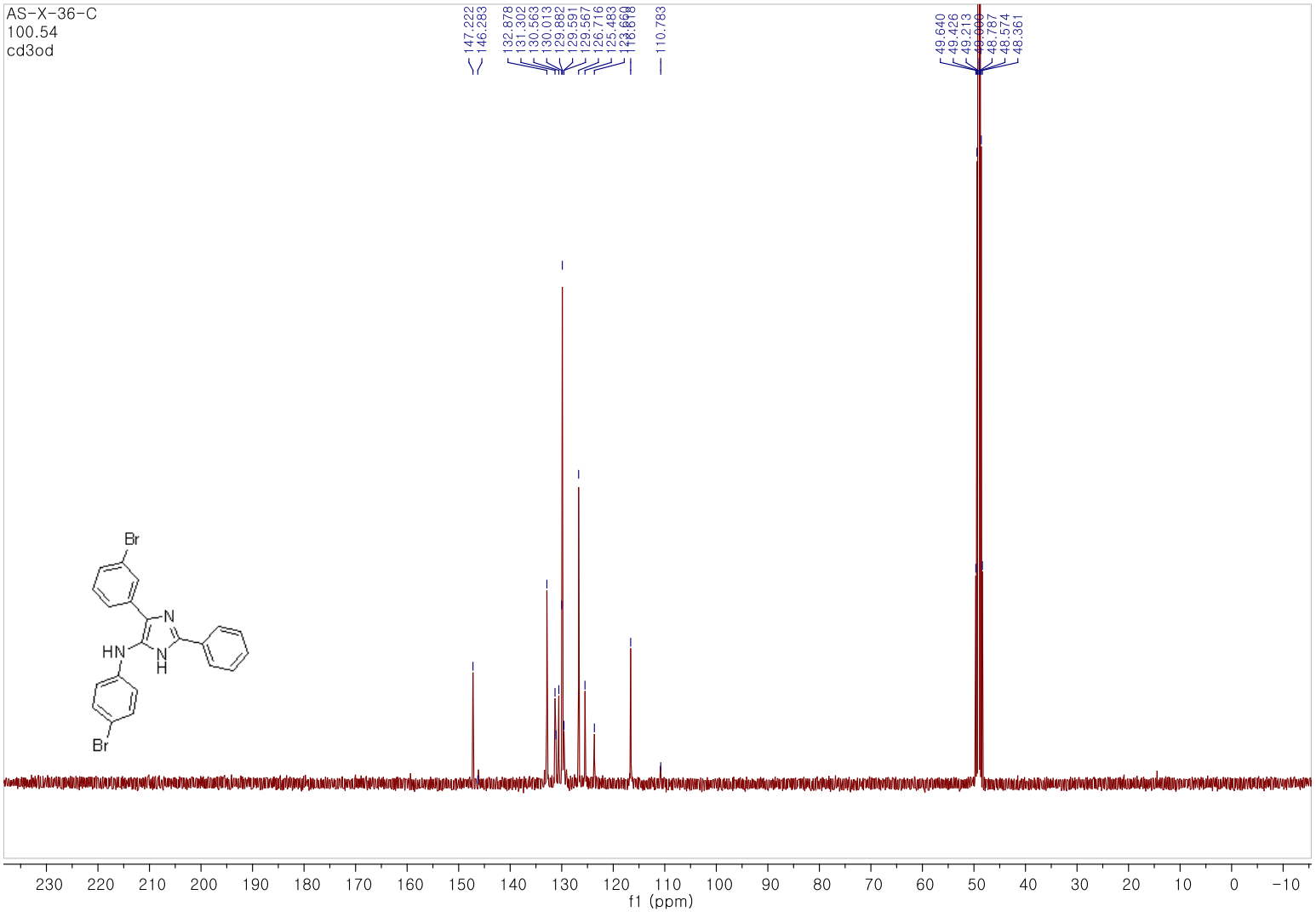
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4v**



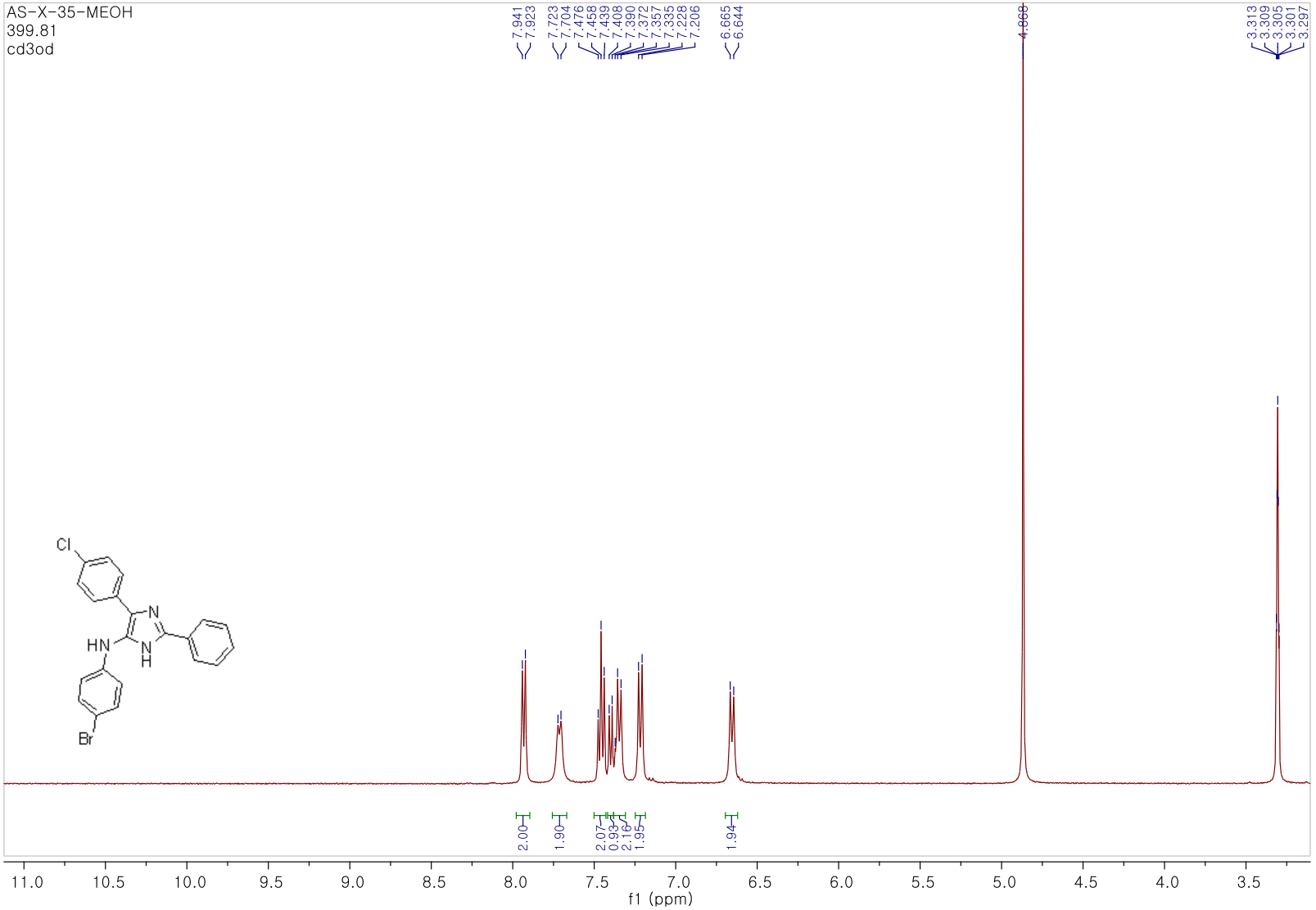
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4w**



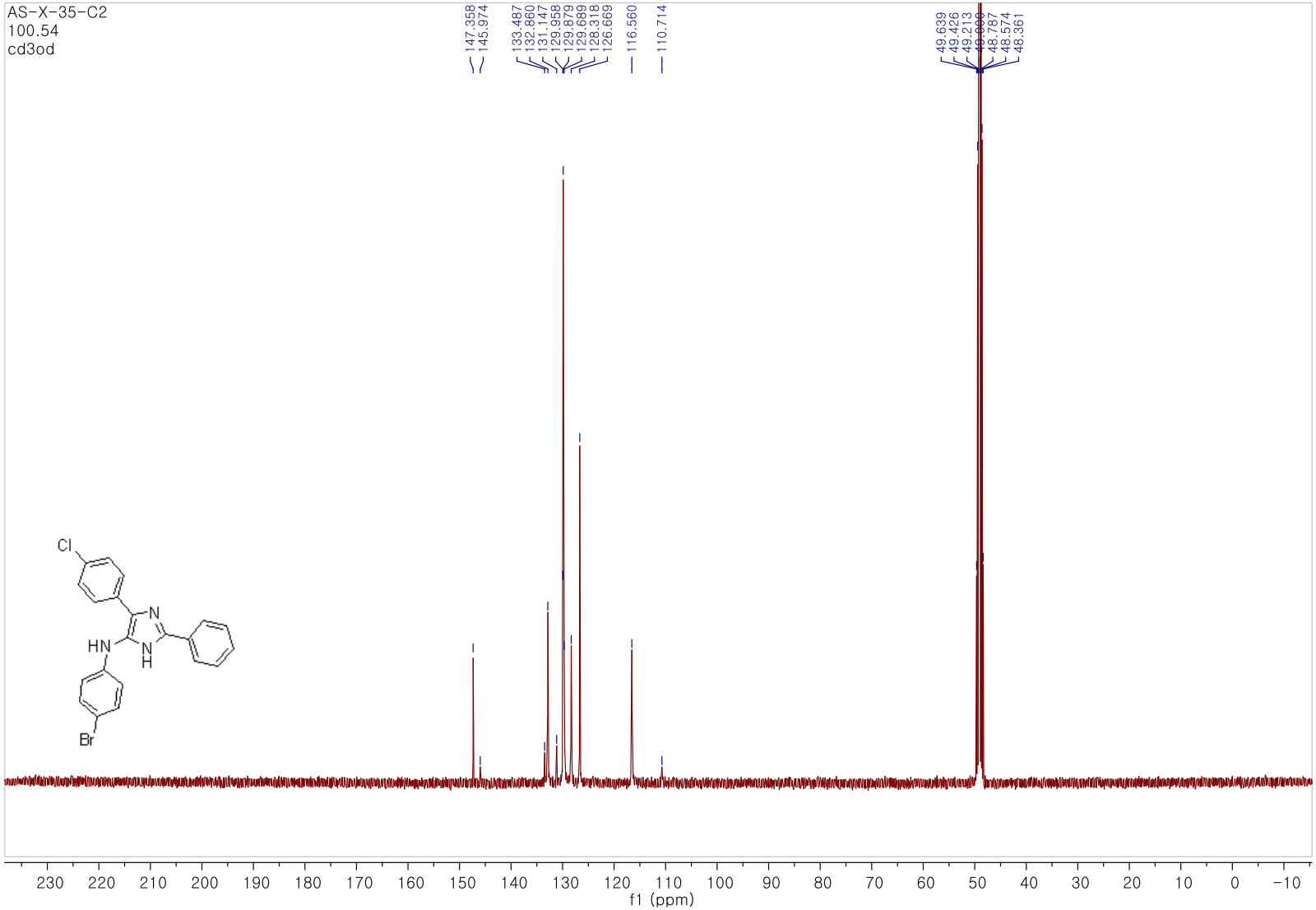
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4w**



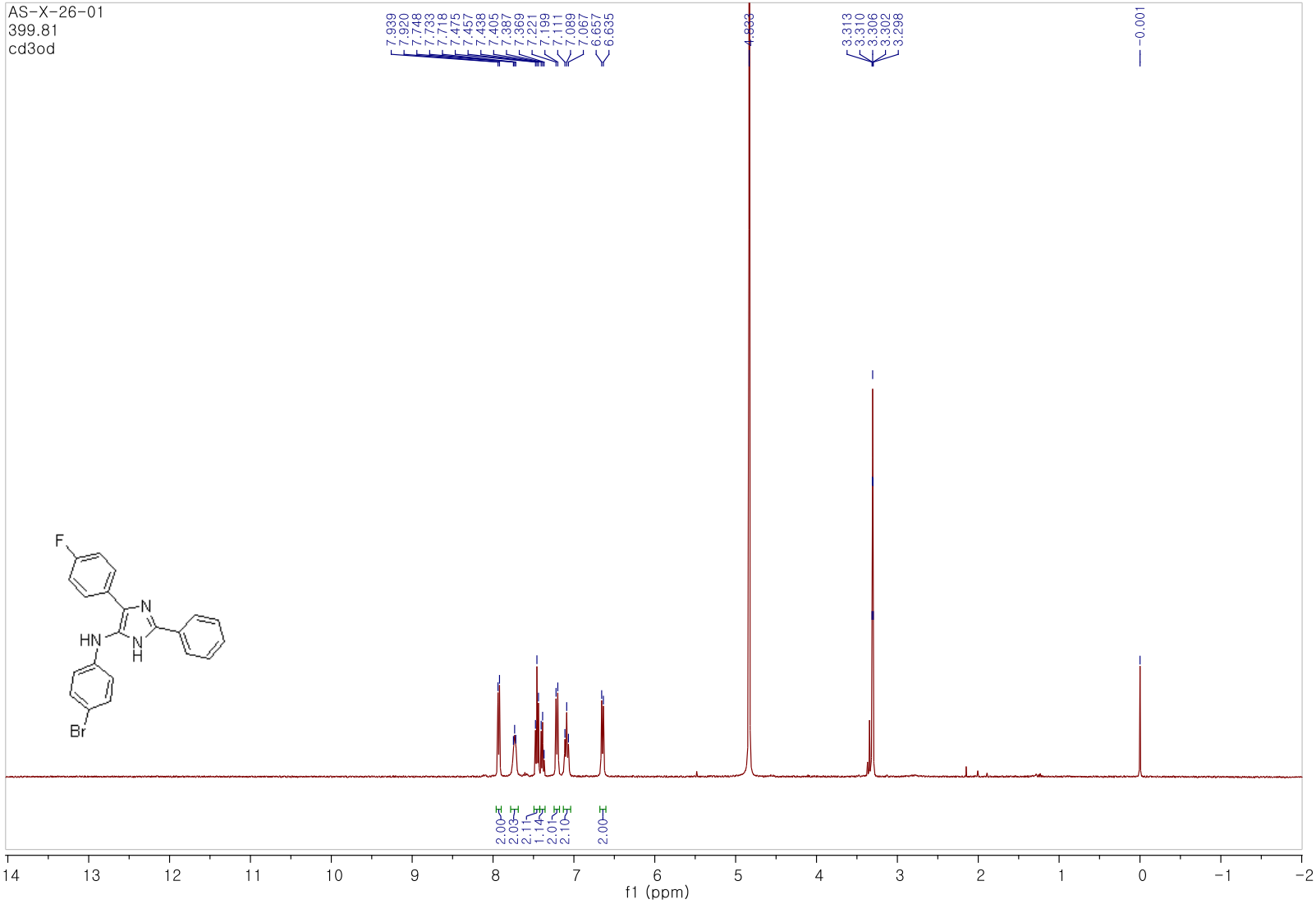
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4x**



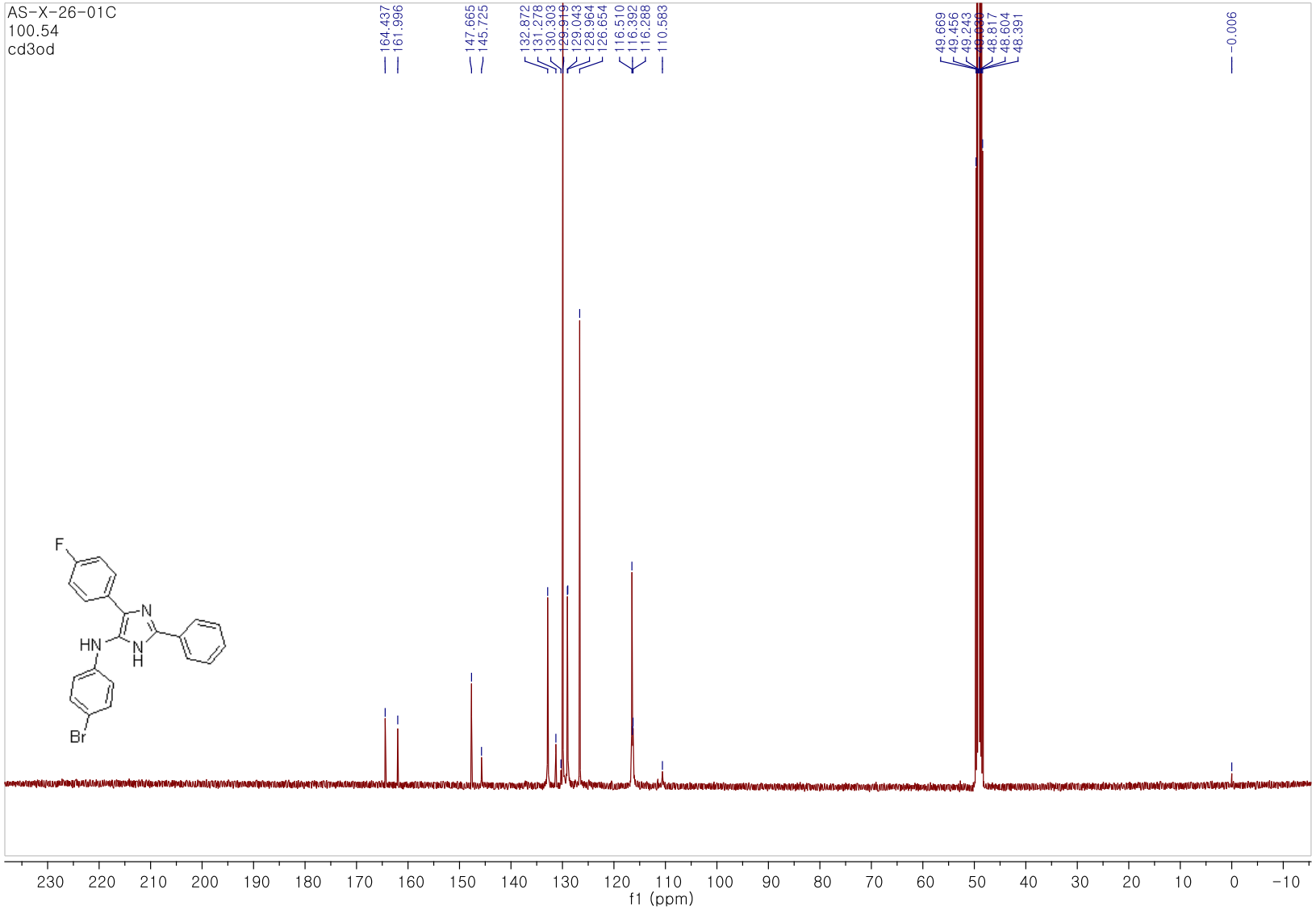
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4x**



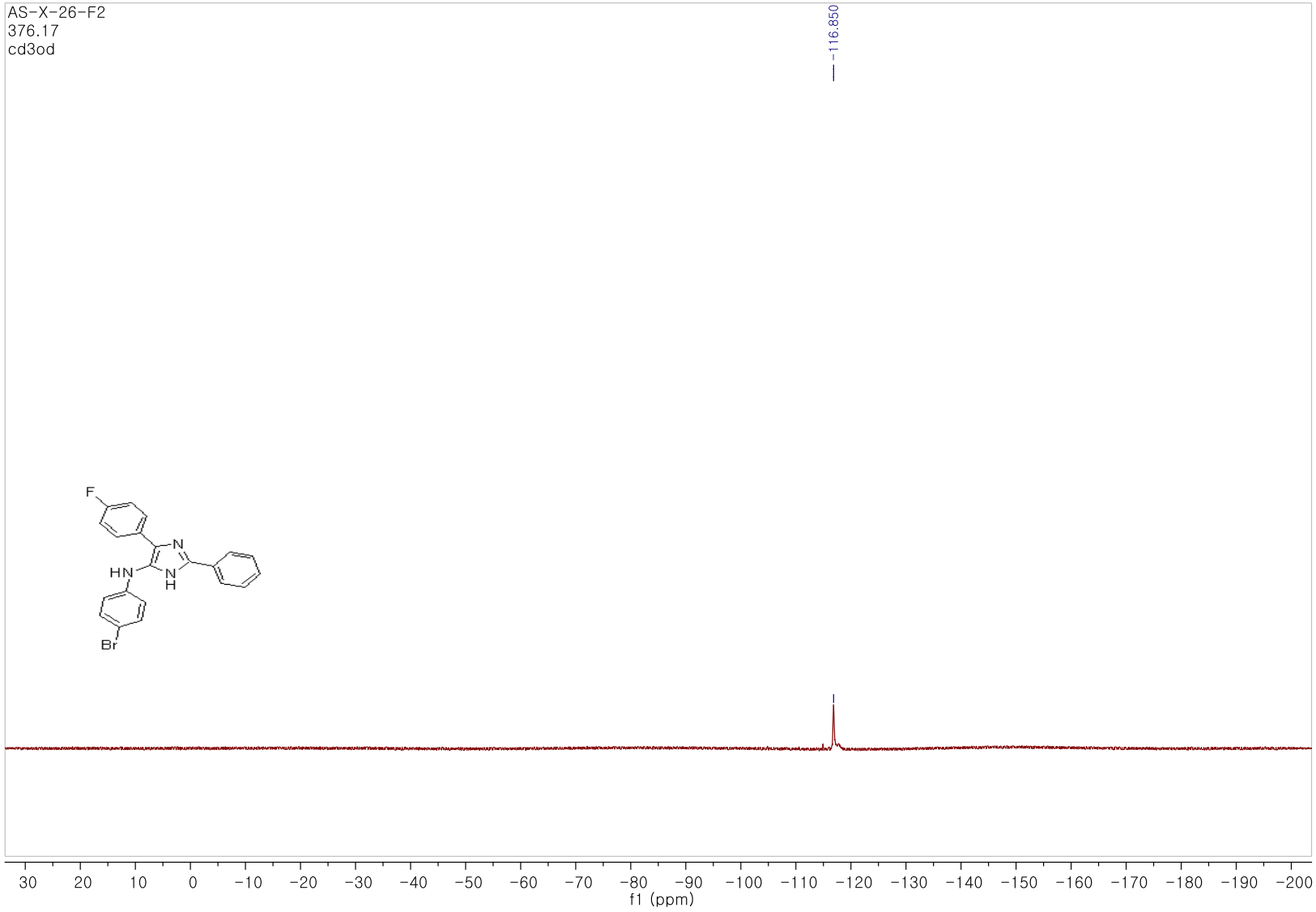
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4y**



^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4y**

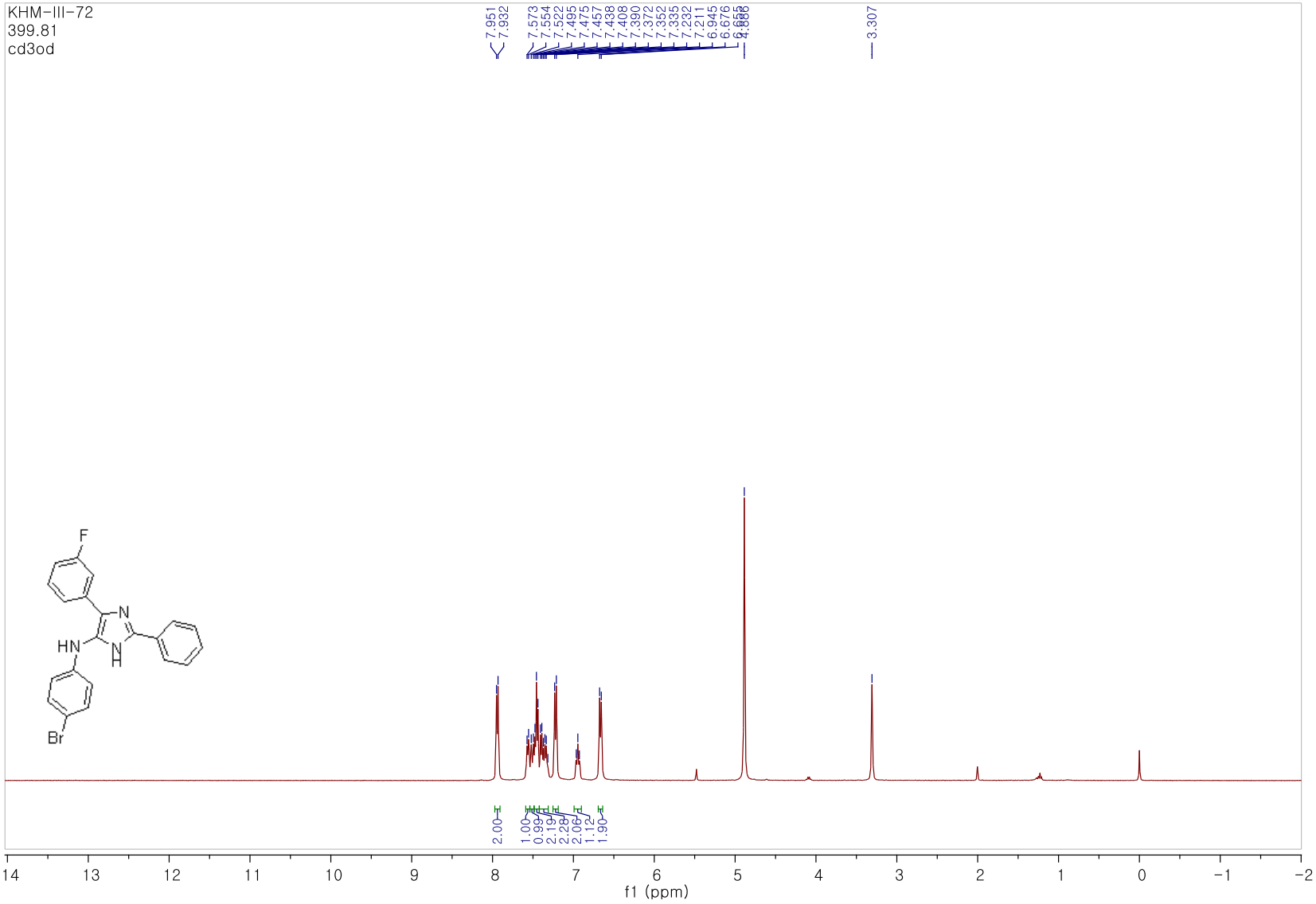


^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4y**

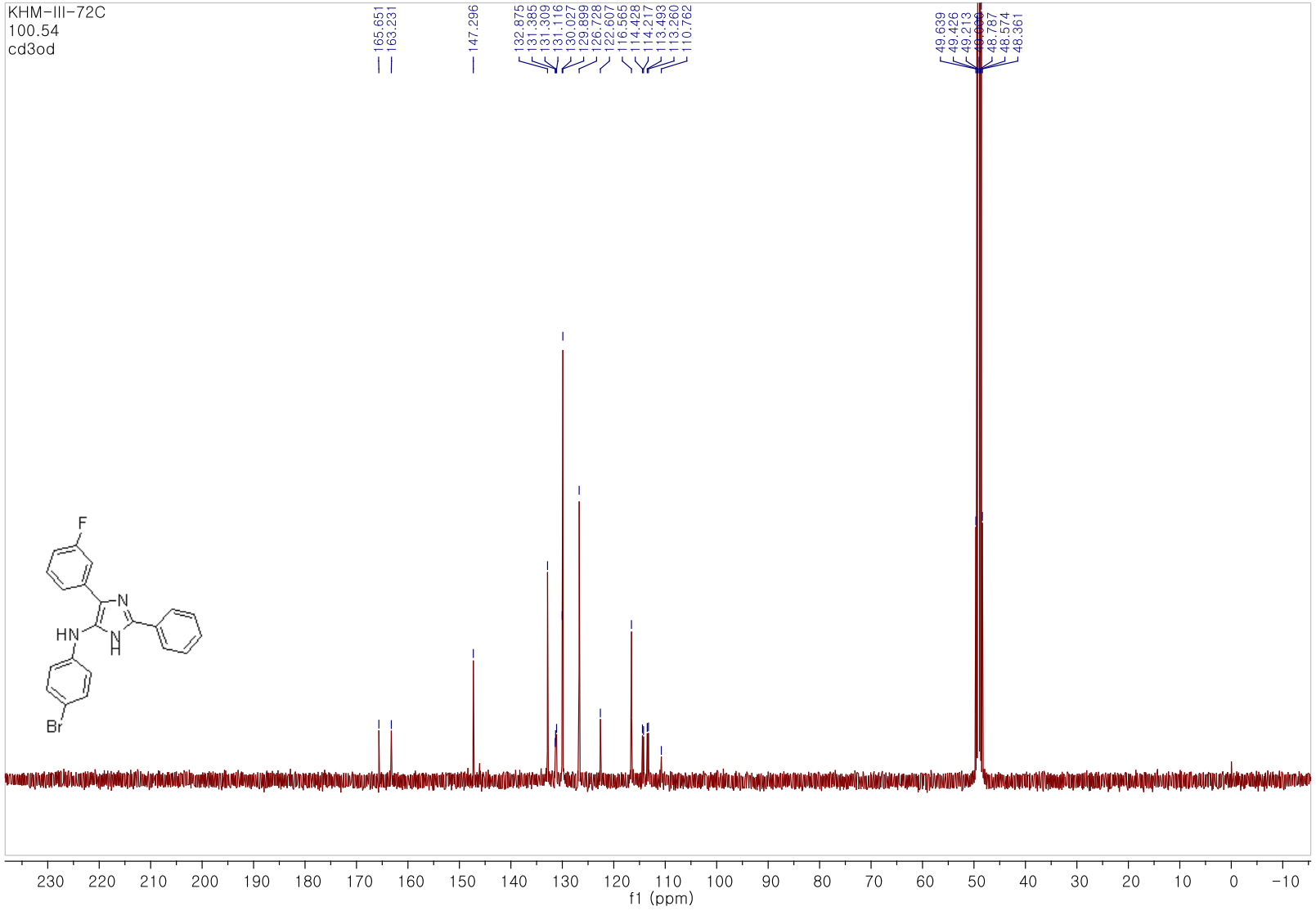


^{1}H NMR (400

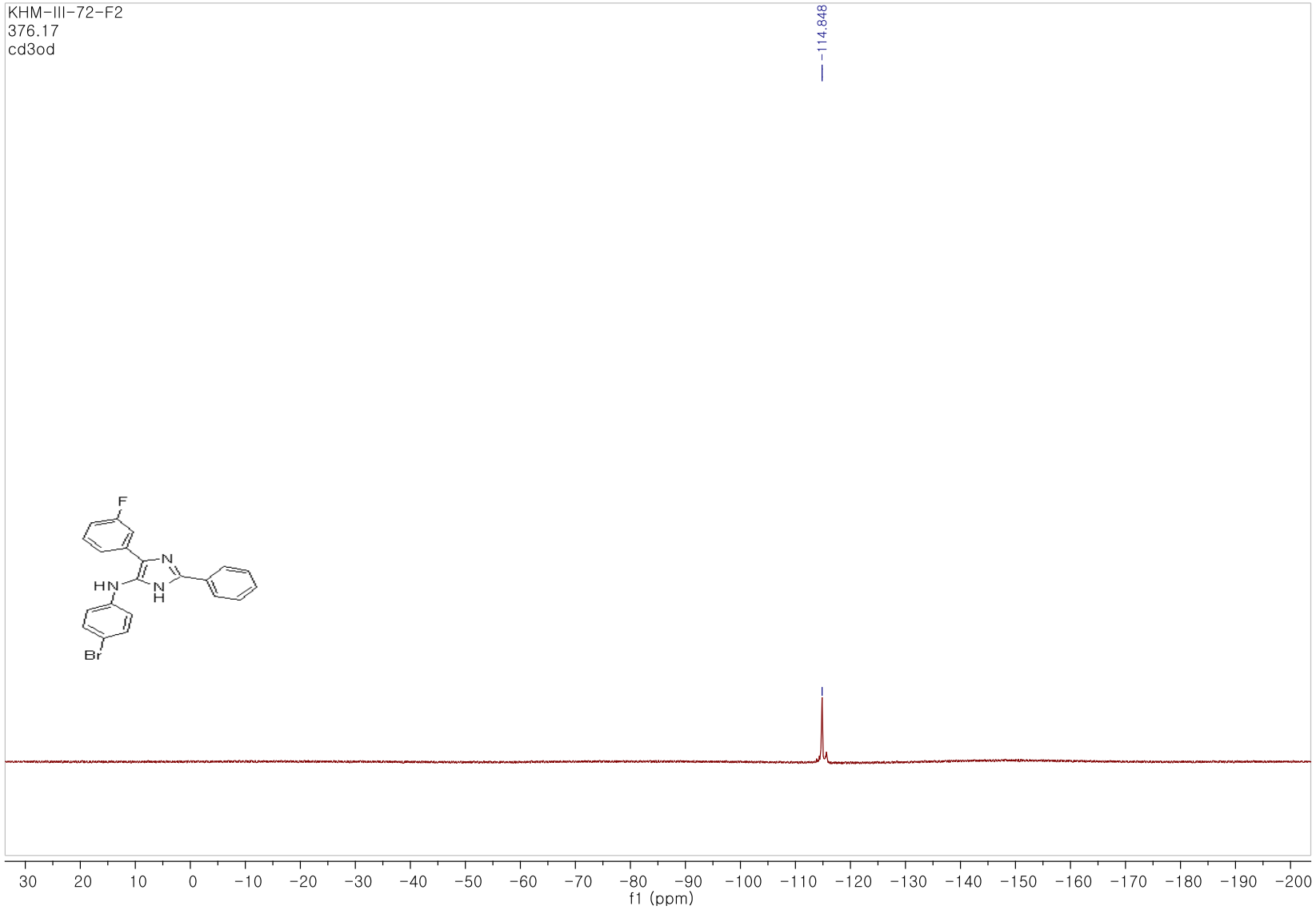
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4z**



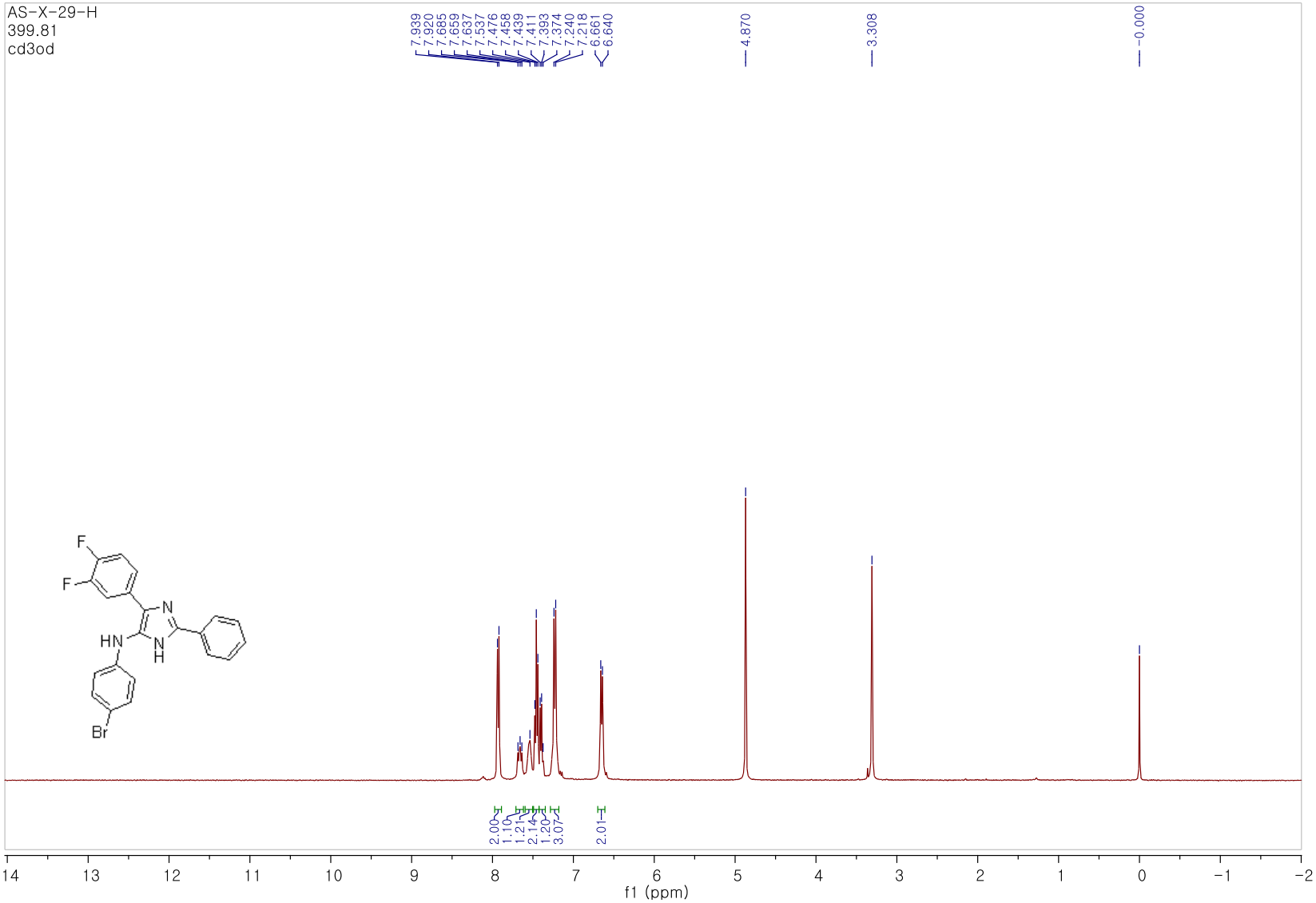
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4z**



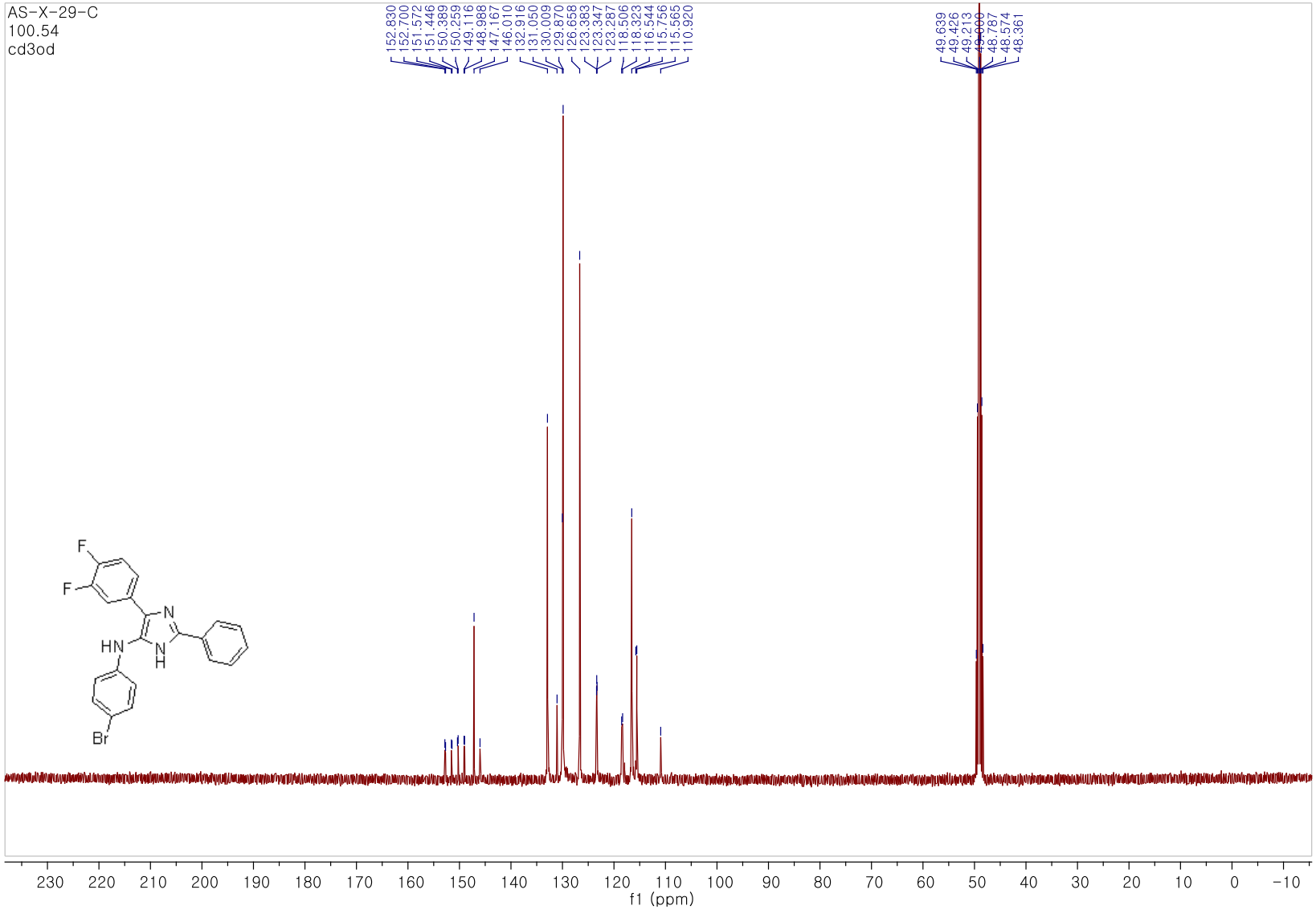
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4z**



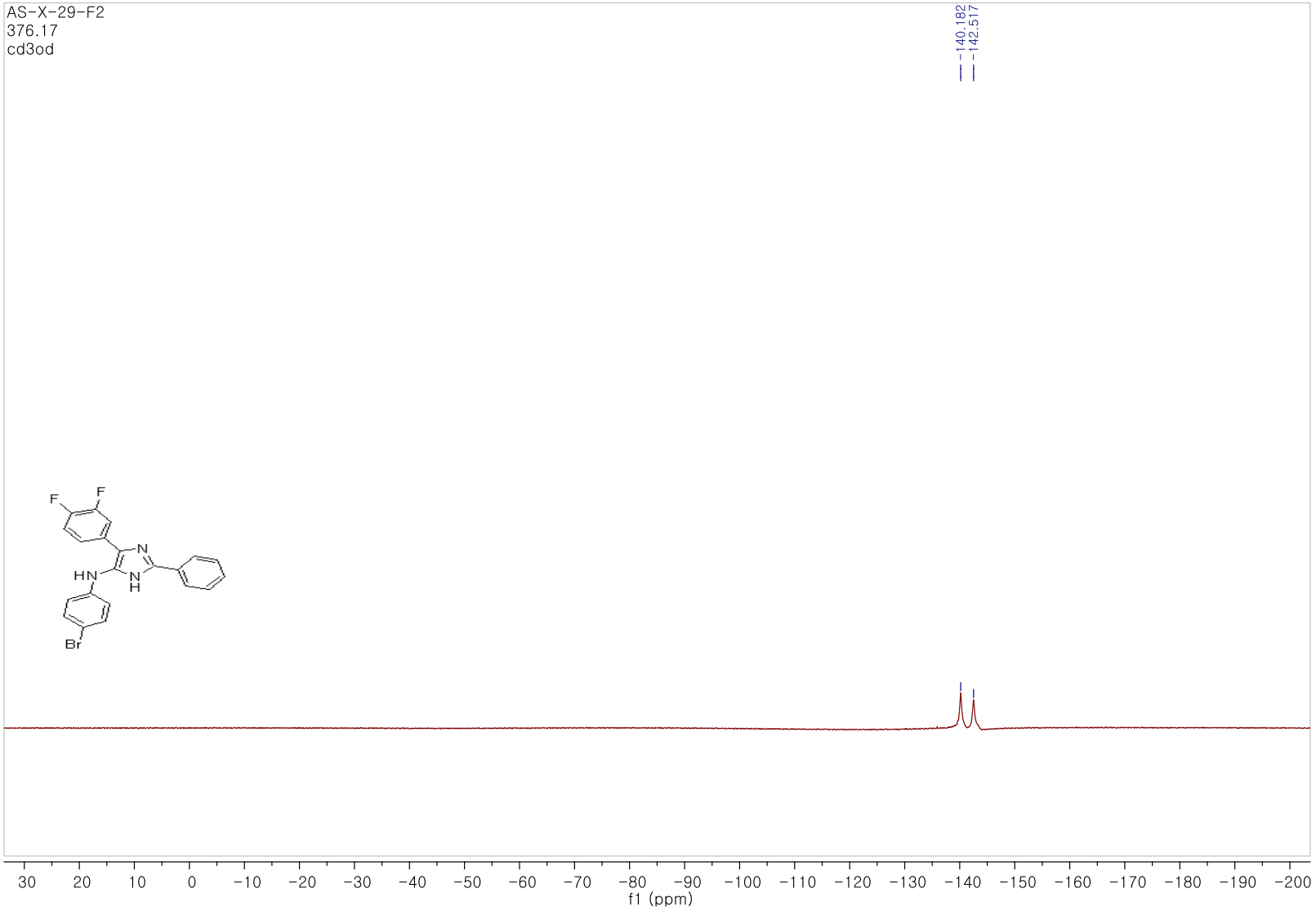
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4aa**



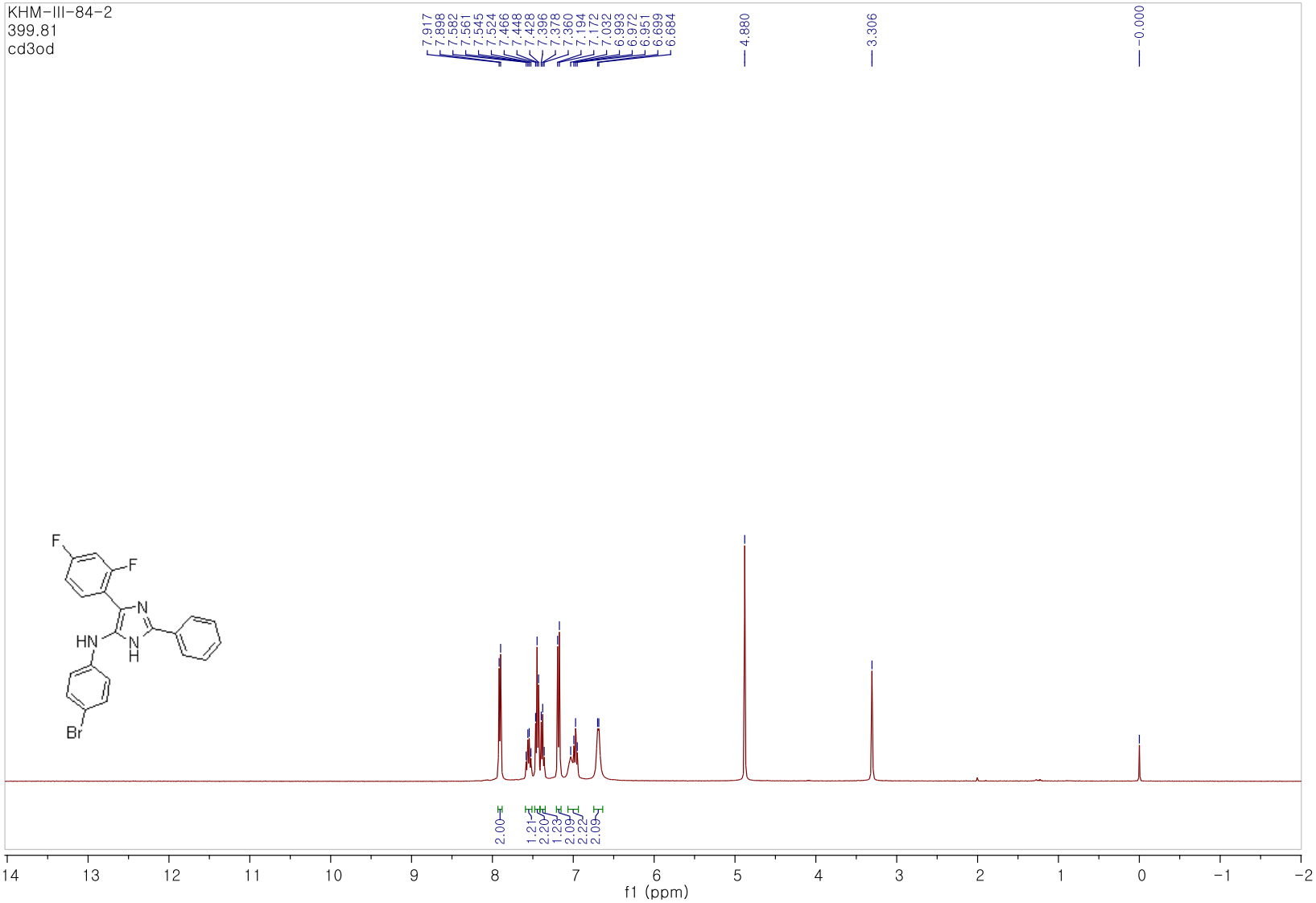
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4aa**



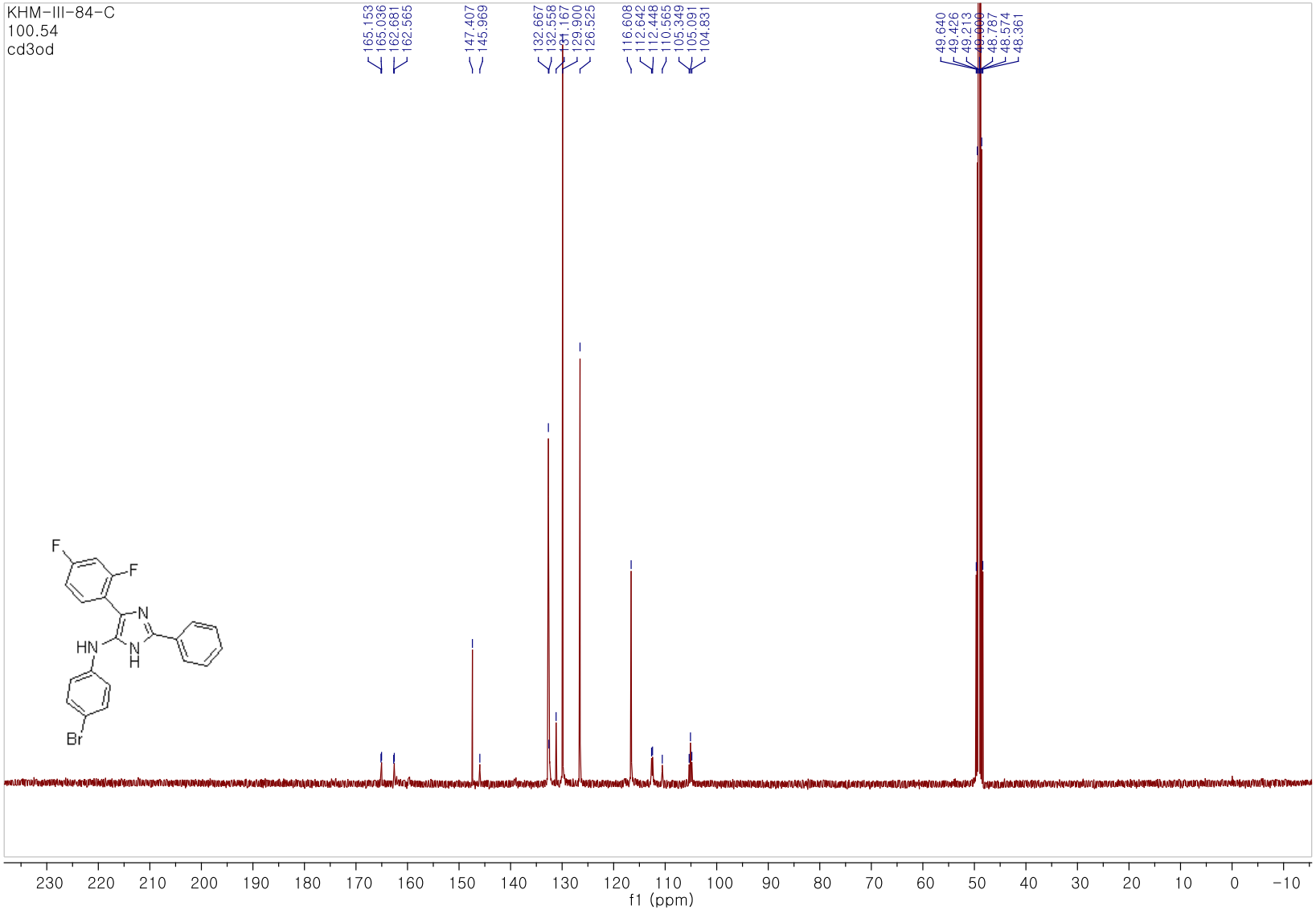
^{19}F NMR (376 MHz, methanol-*d*$_4$) spectrum of **4aa**



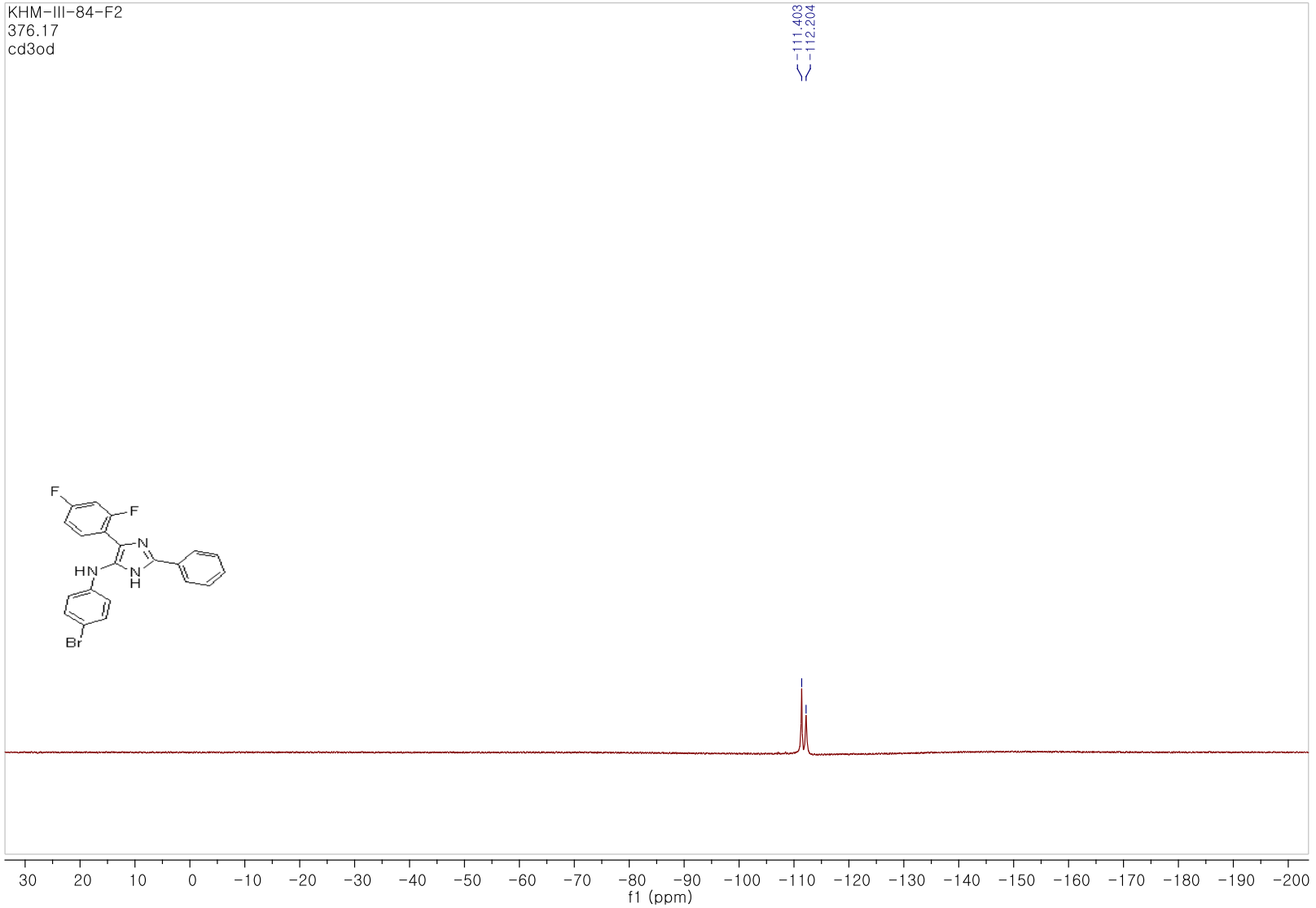
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ab**



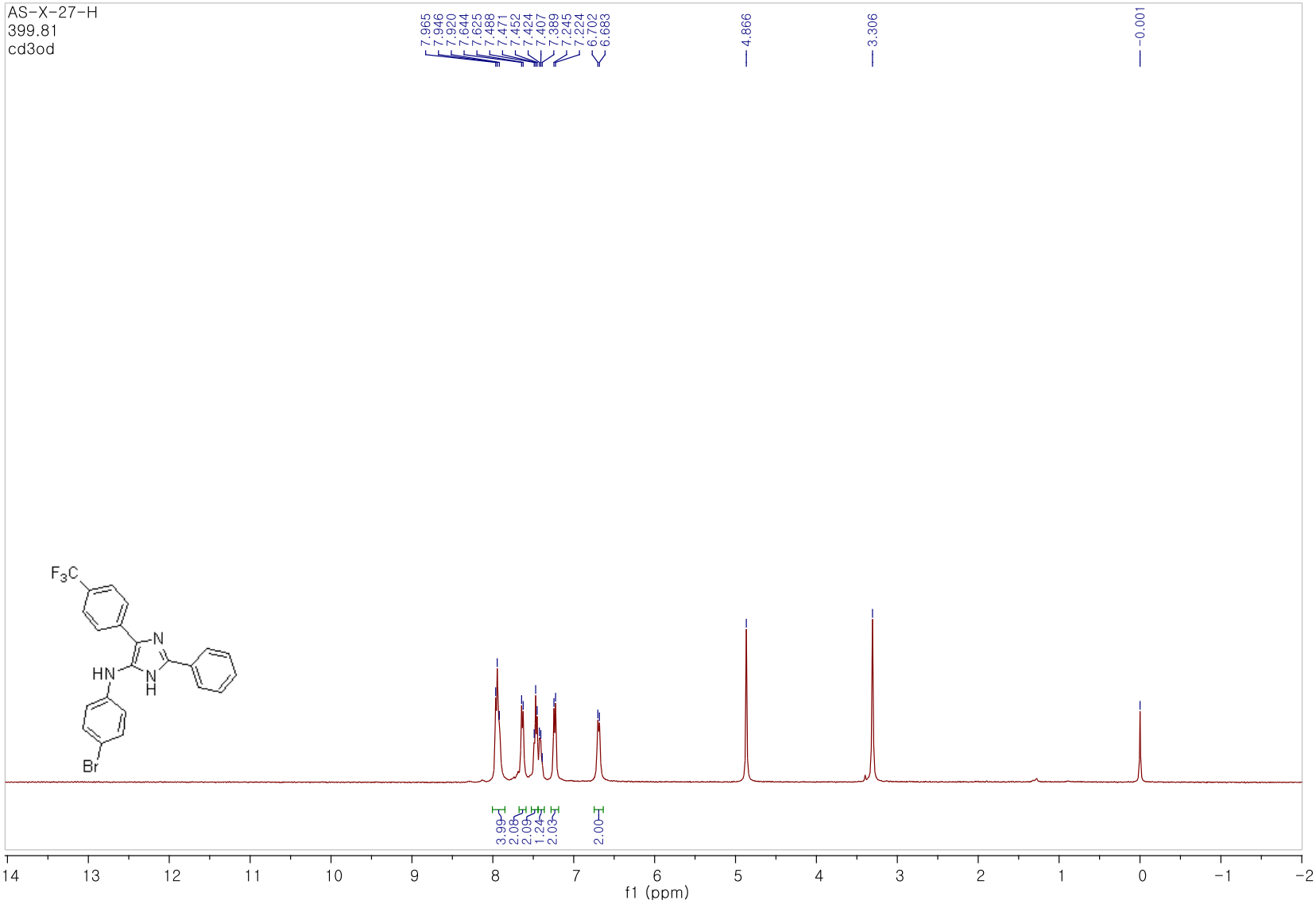
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ab**



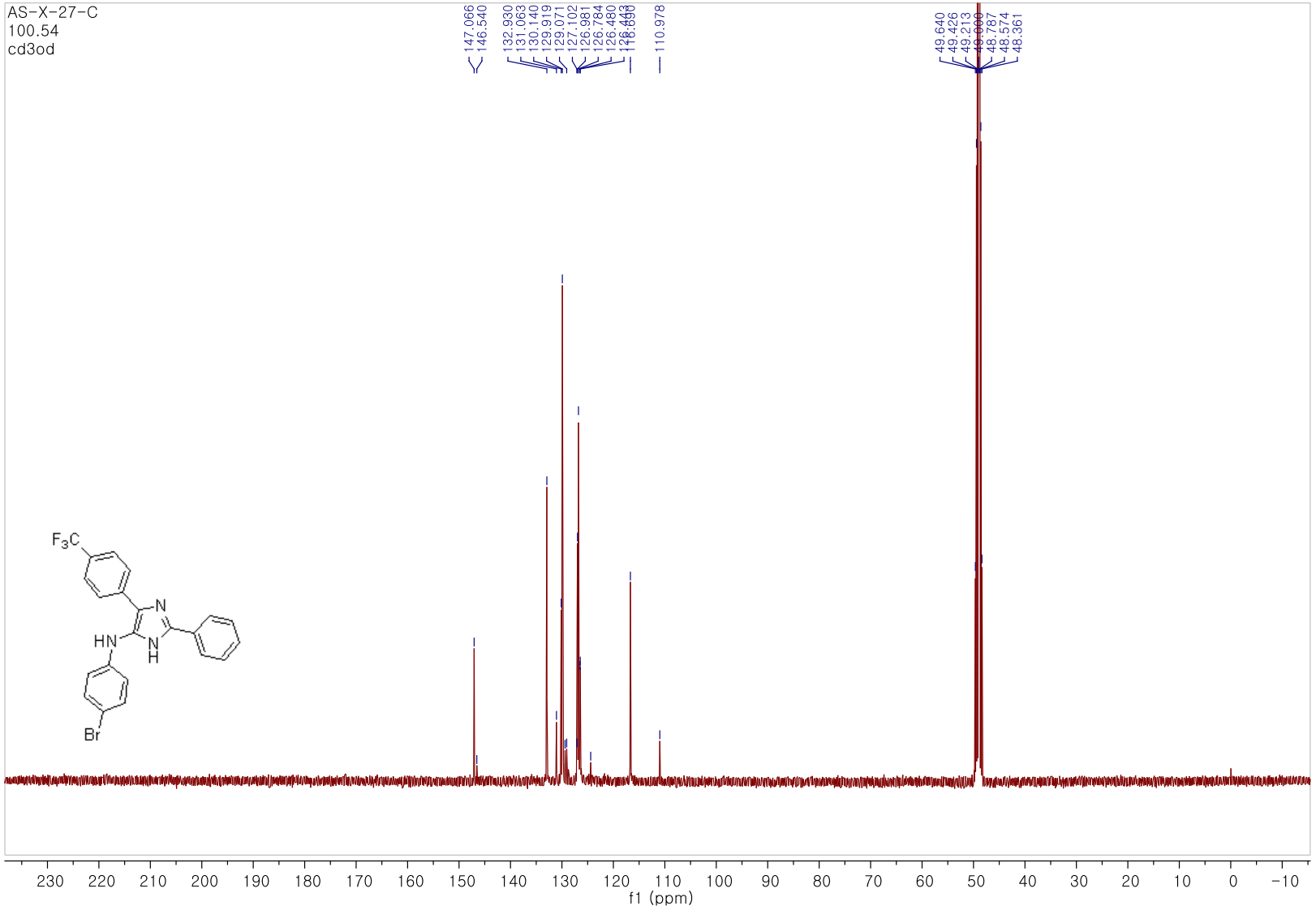
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4ab**



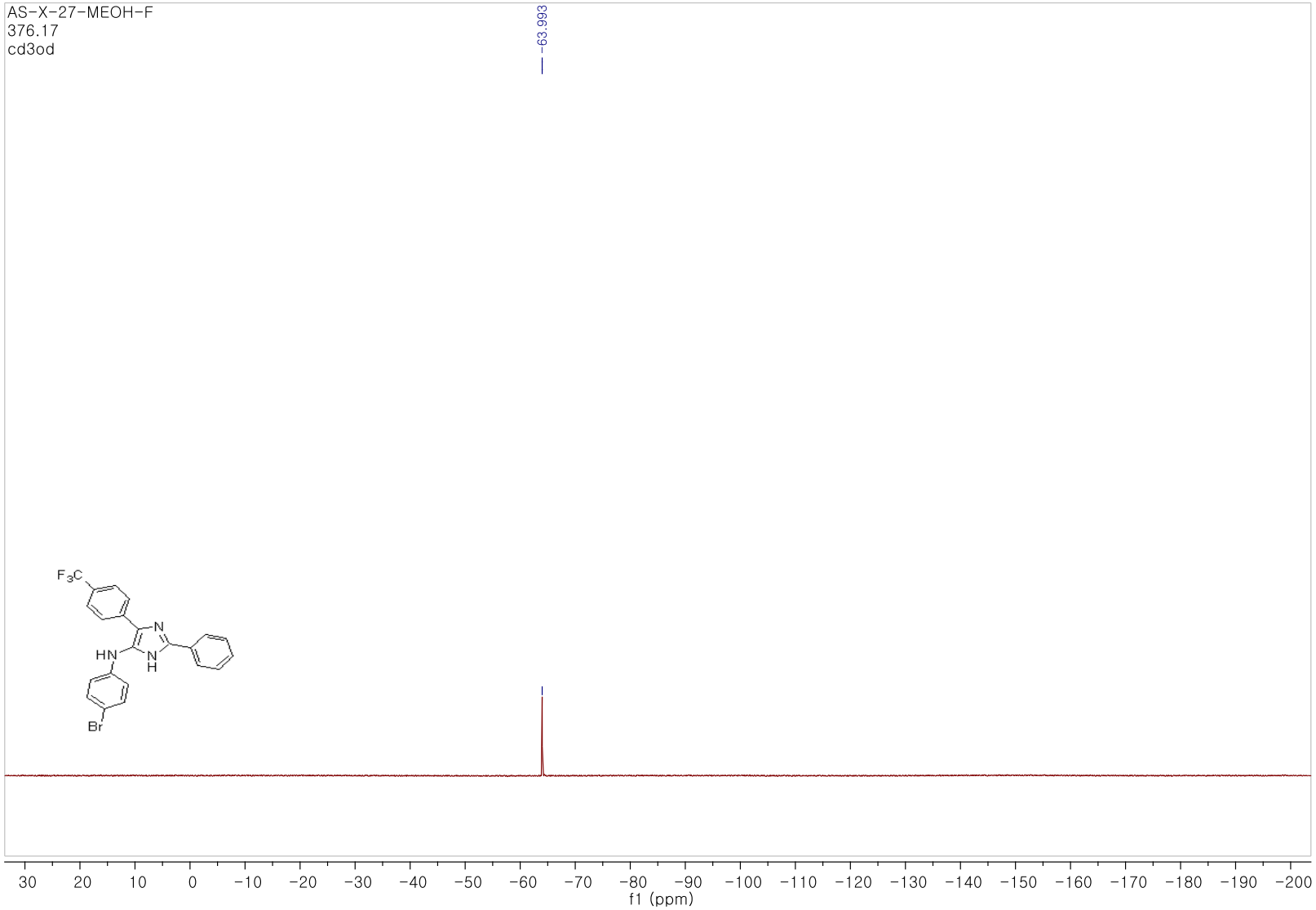
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ac**



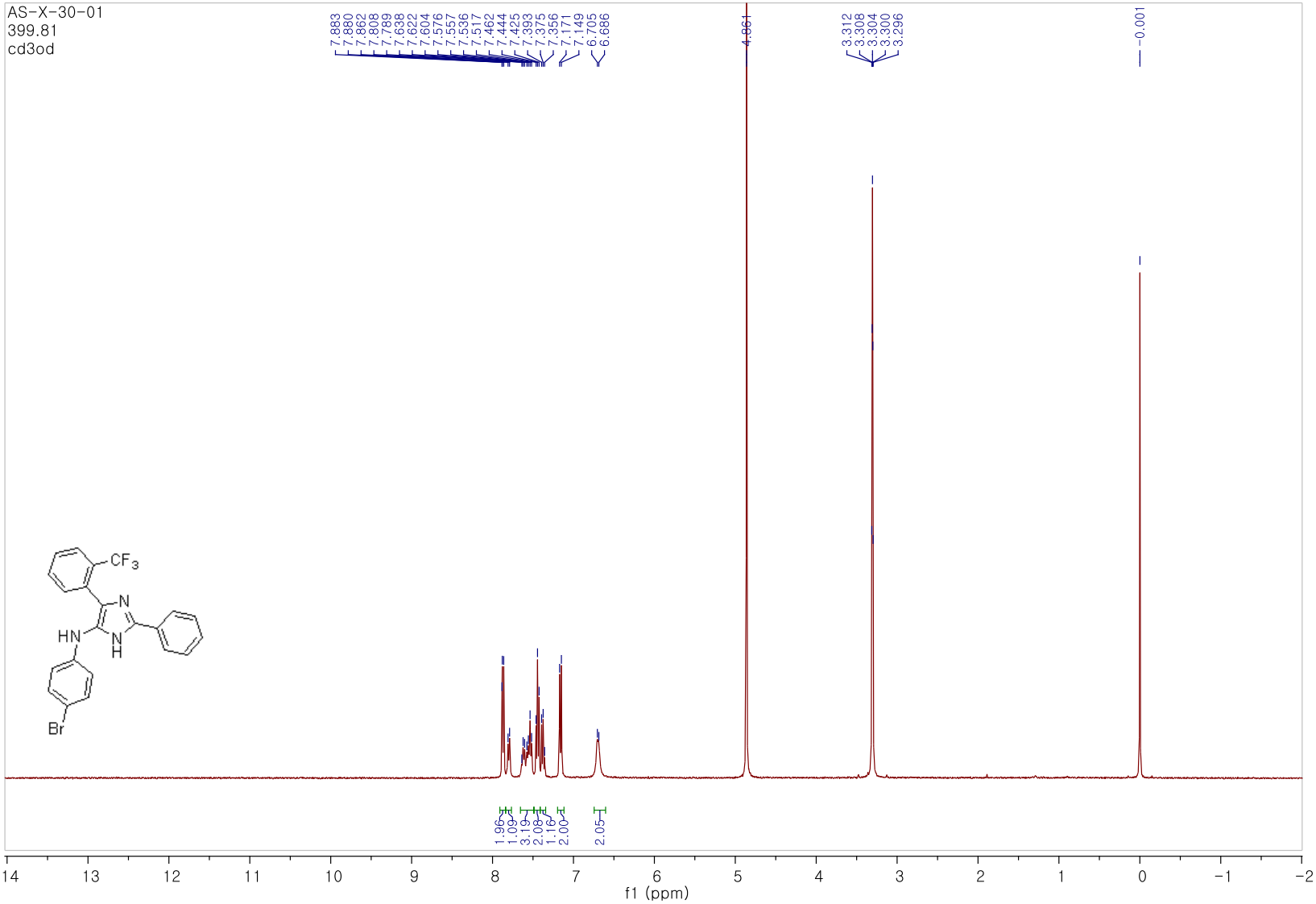
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ac**



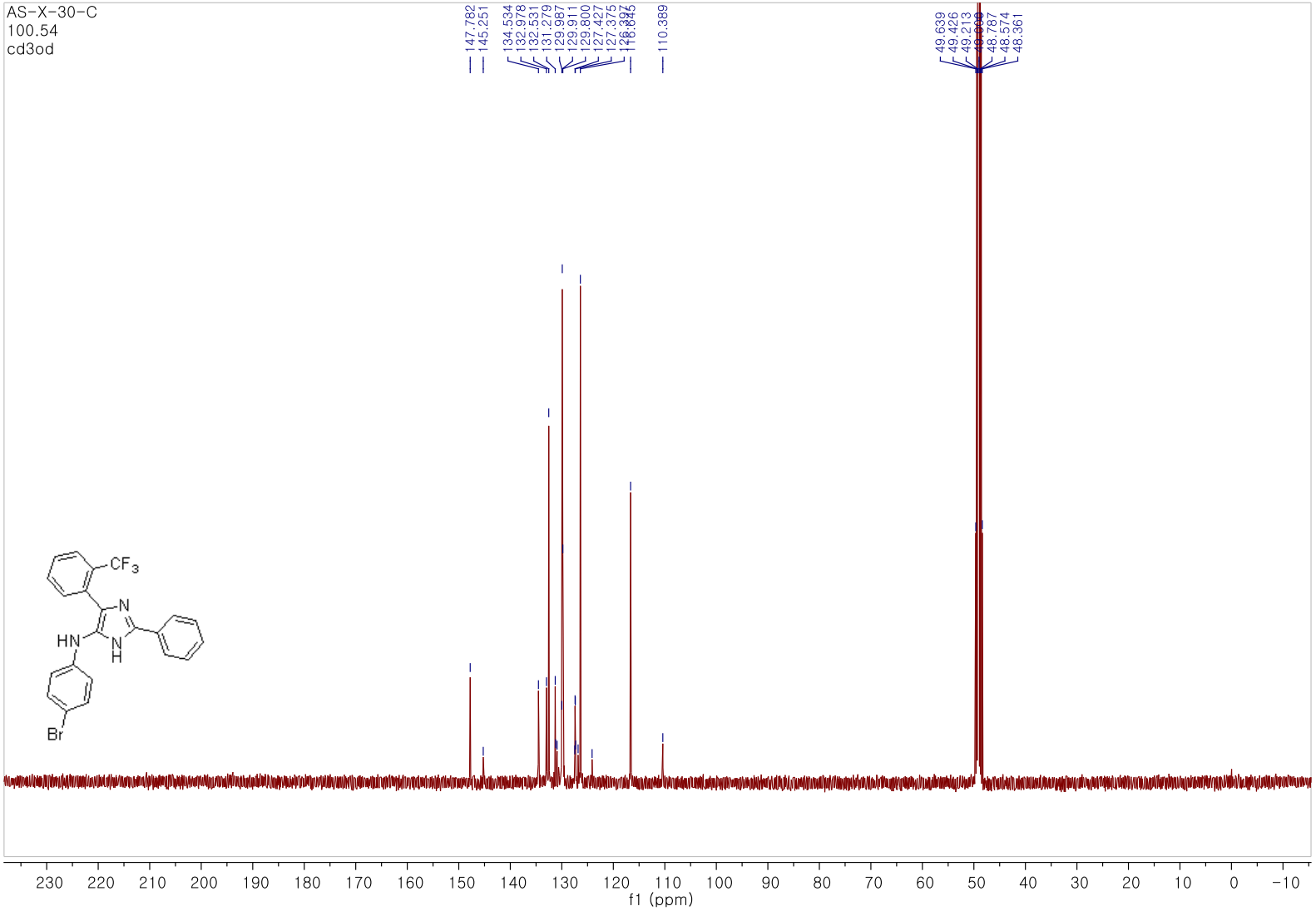
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4ac**



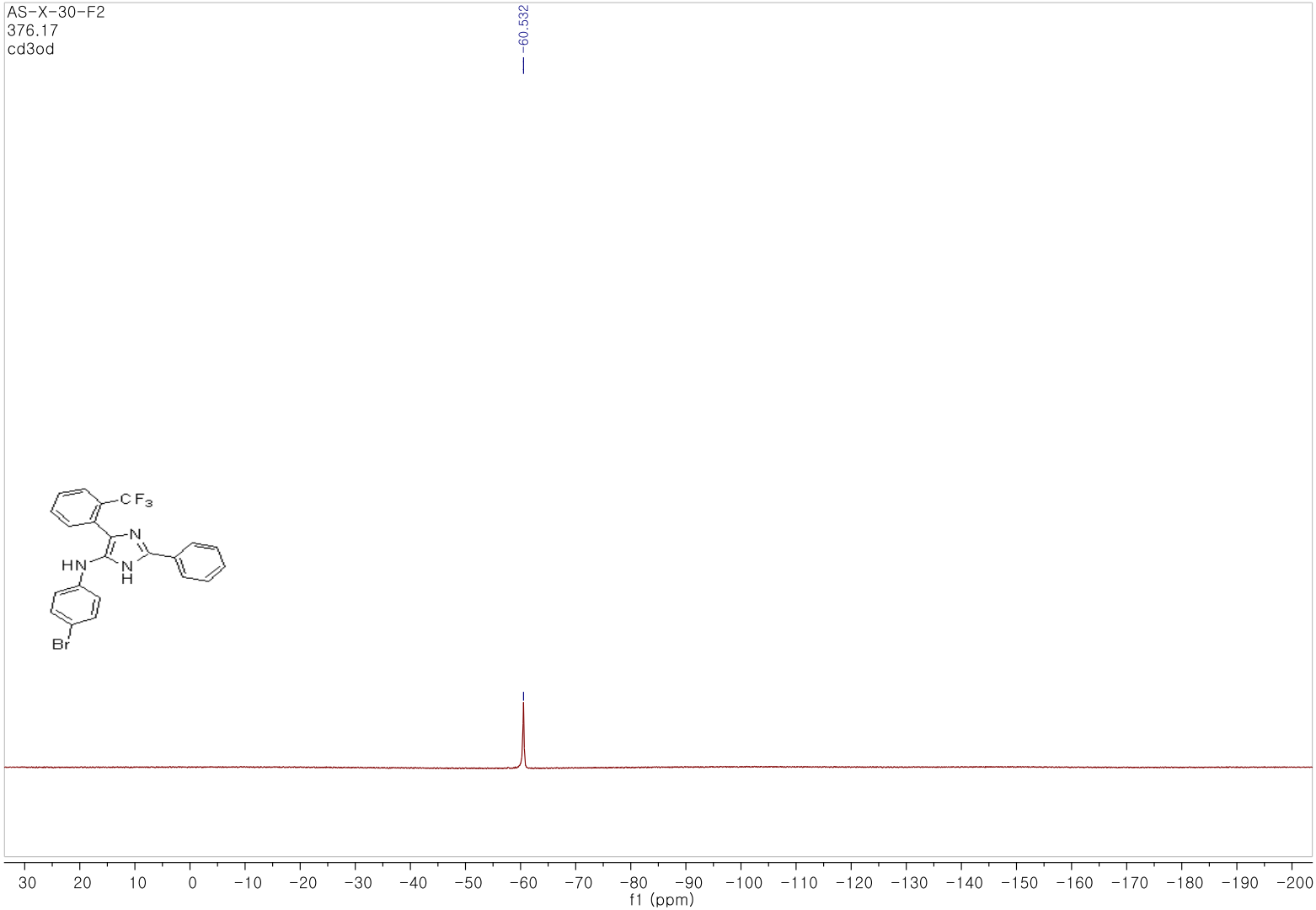
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ad**



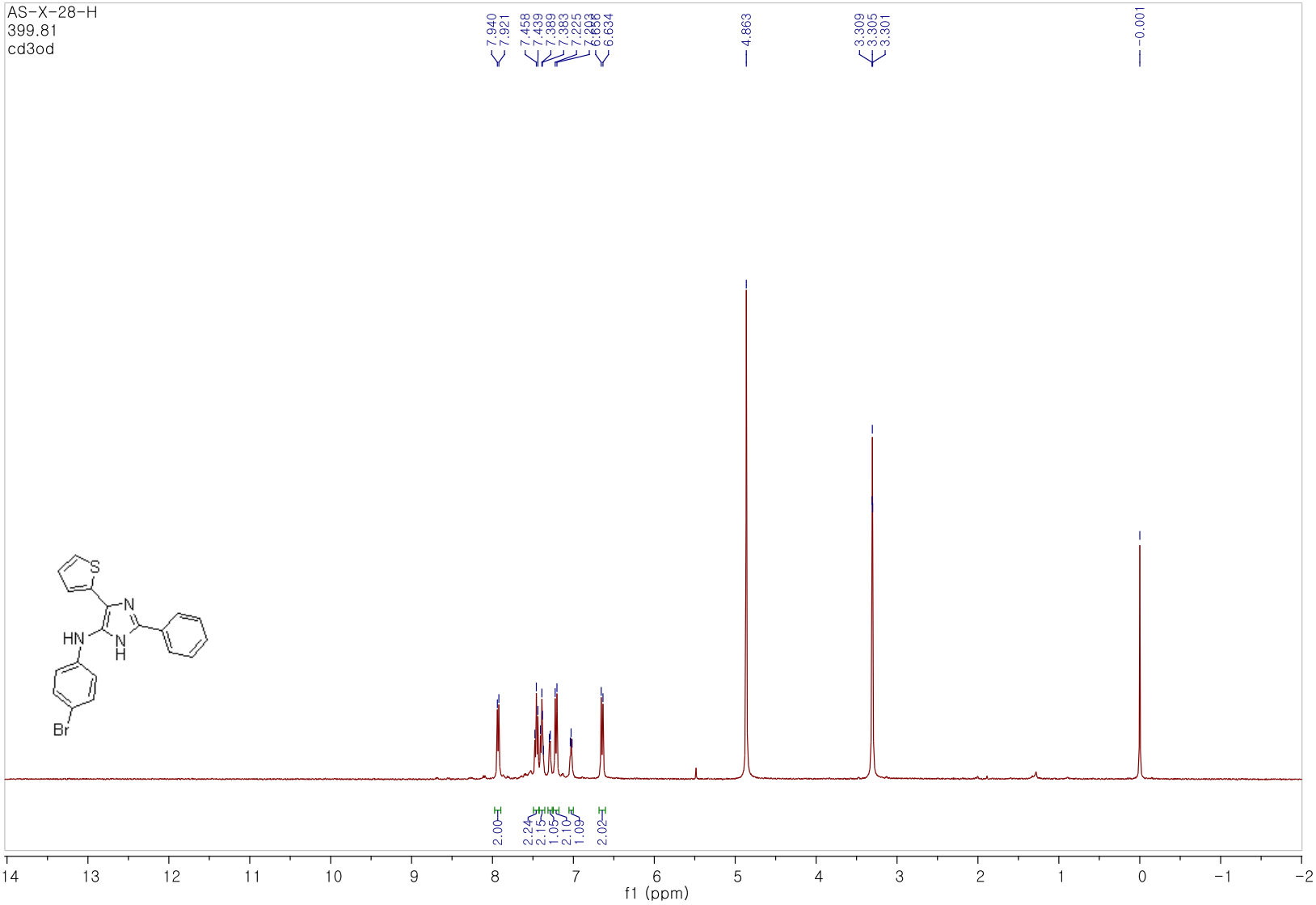
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ad**



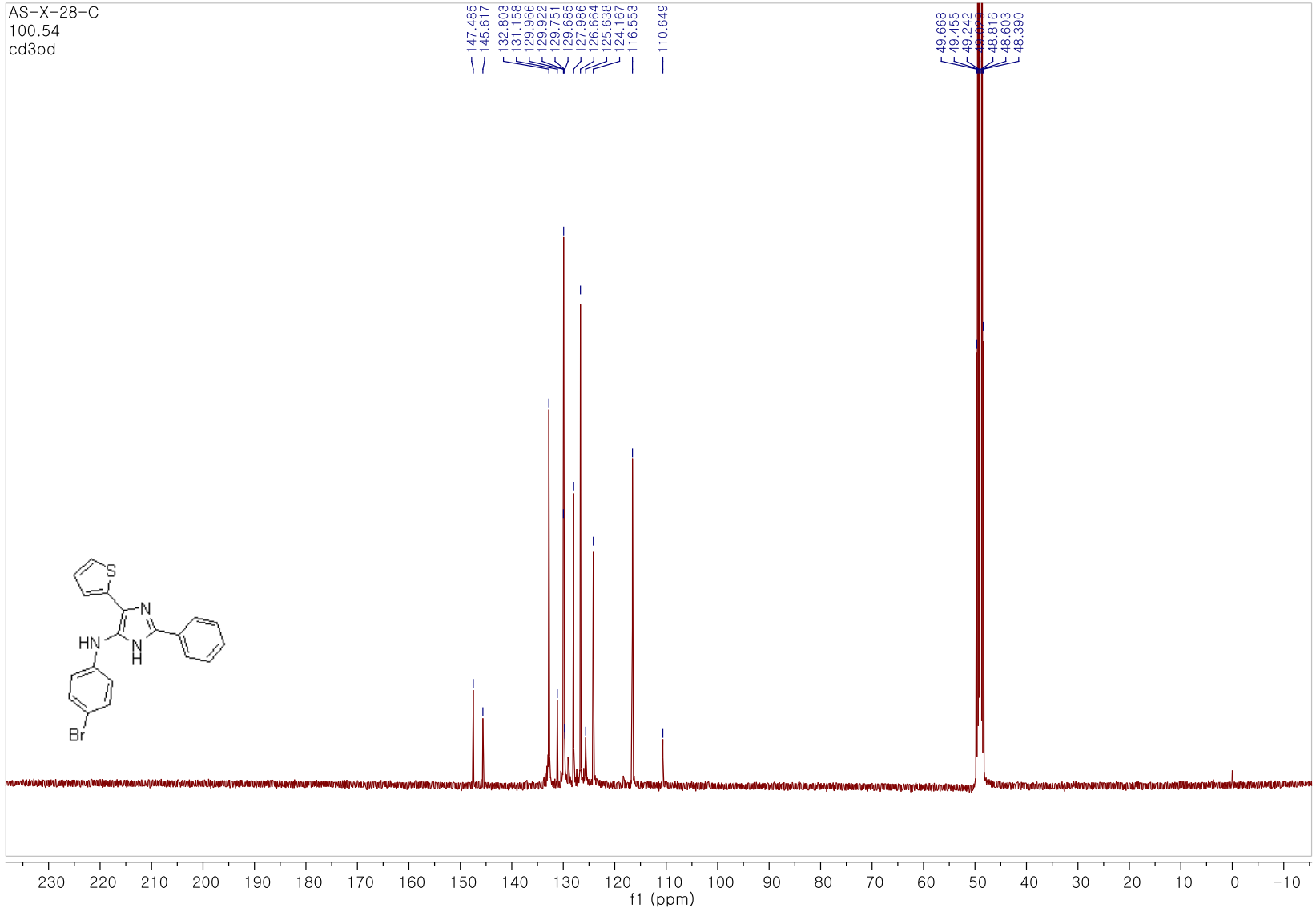
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4ad**



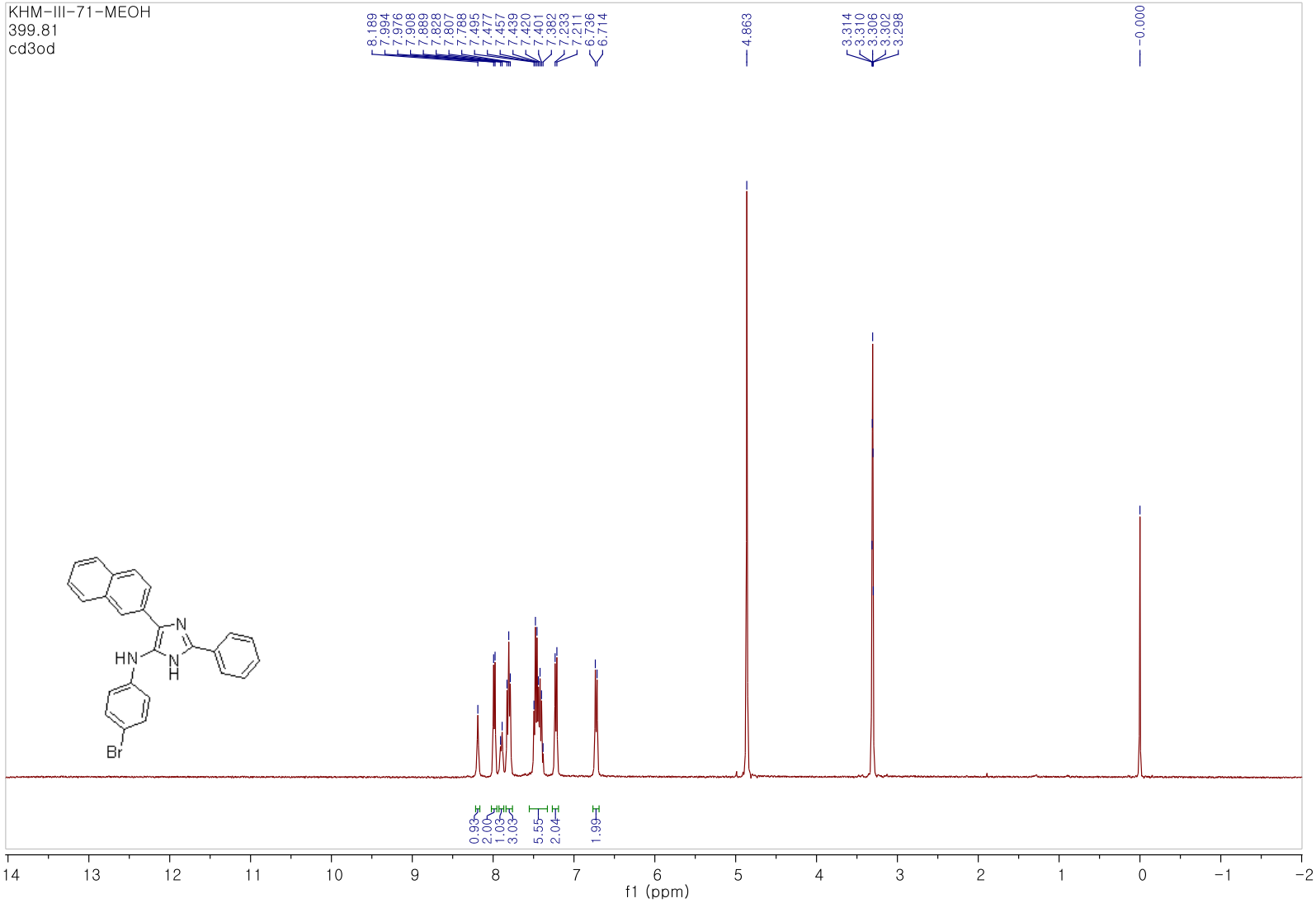
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ae**



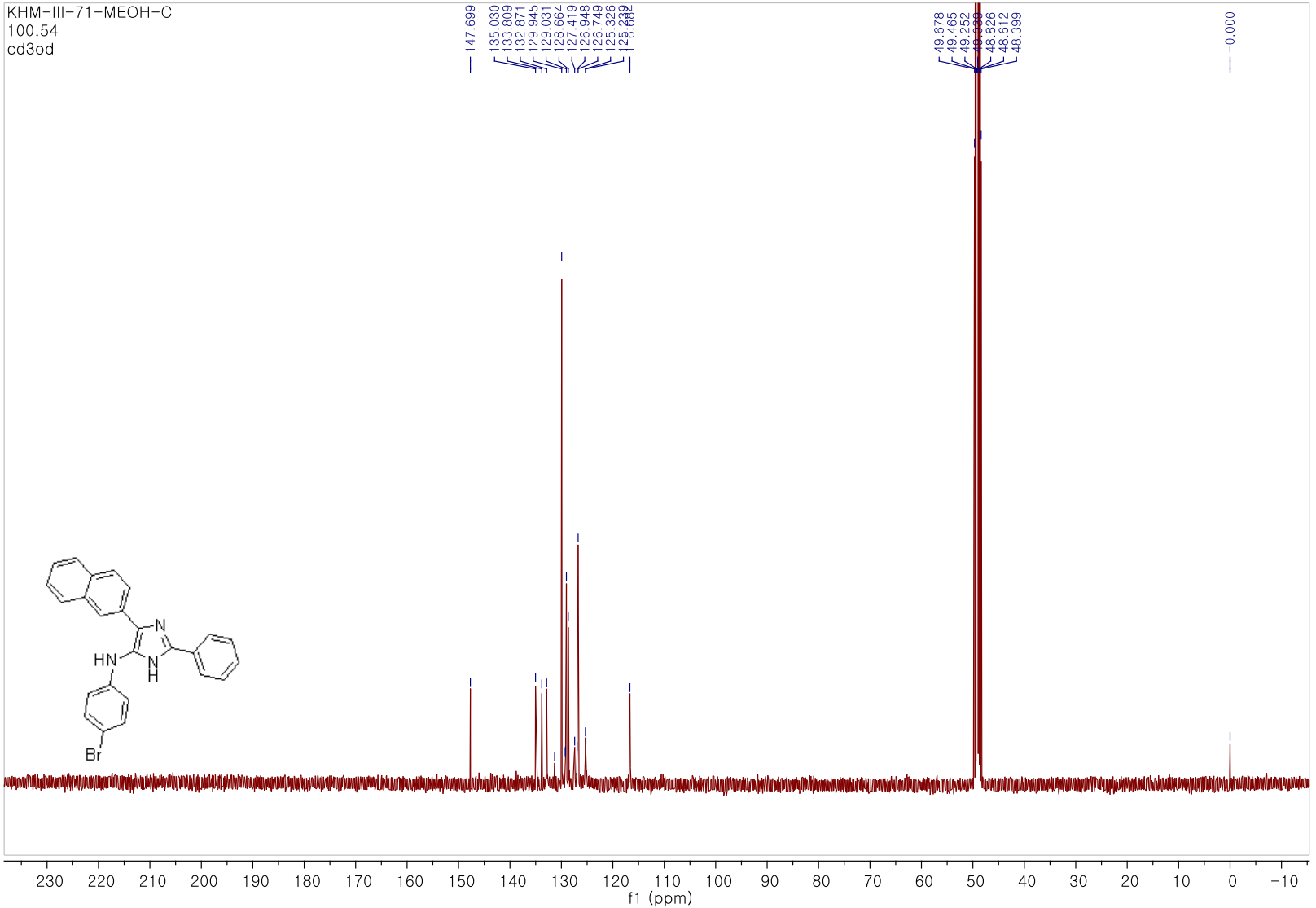
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ae**



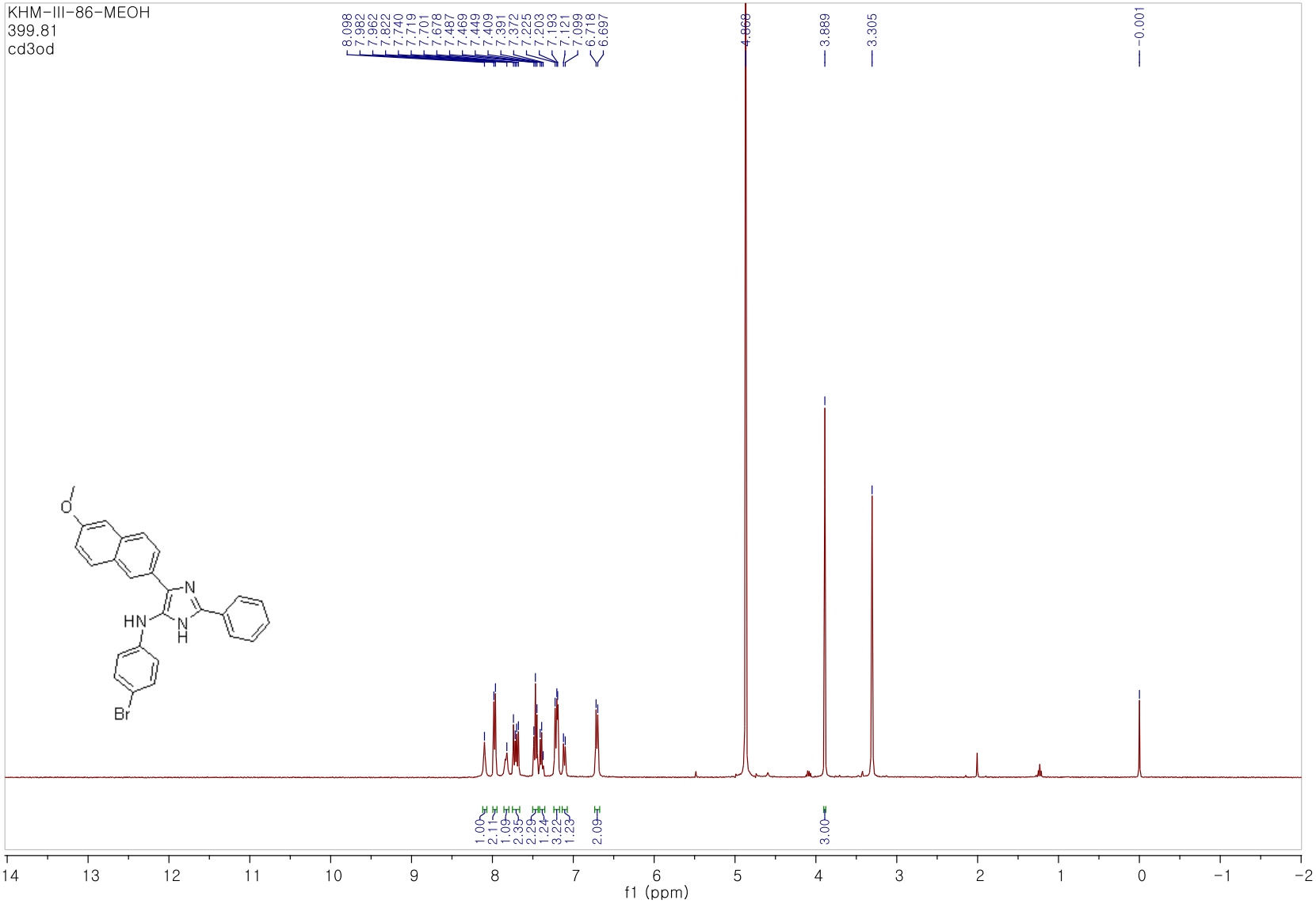
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4af**



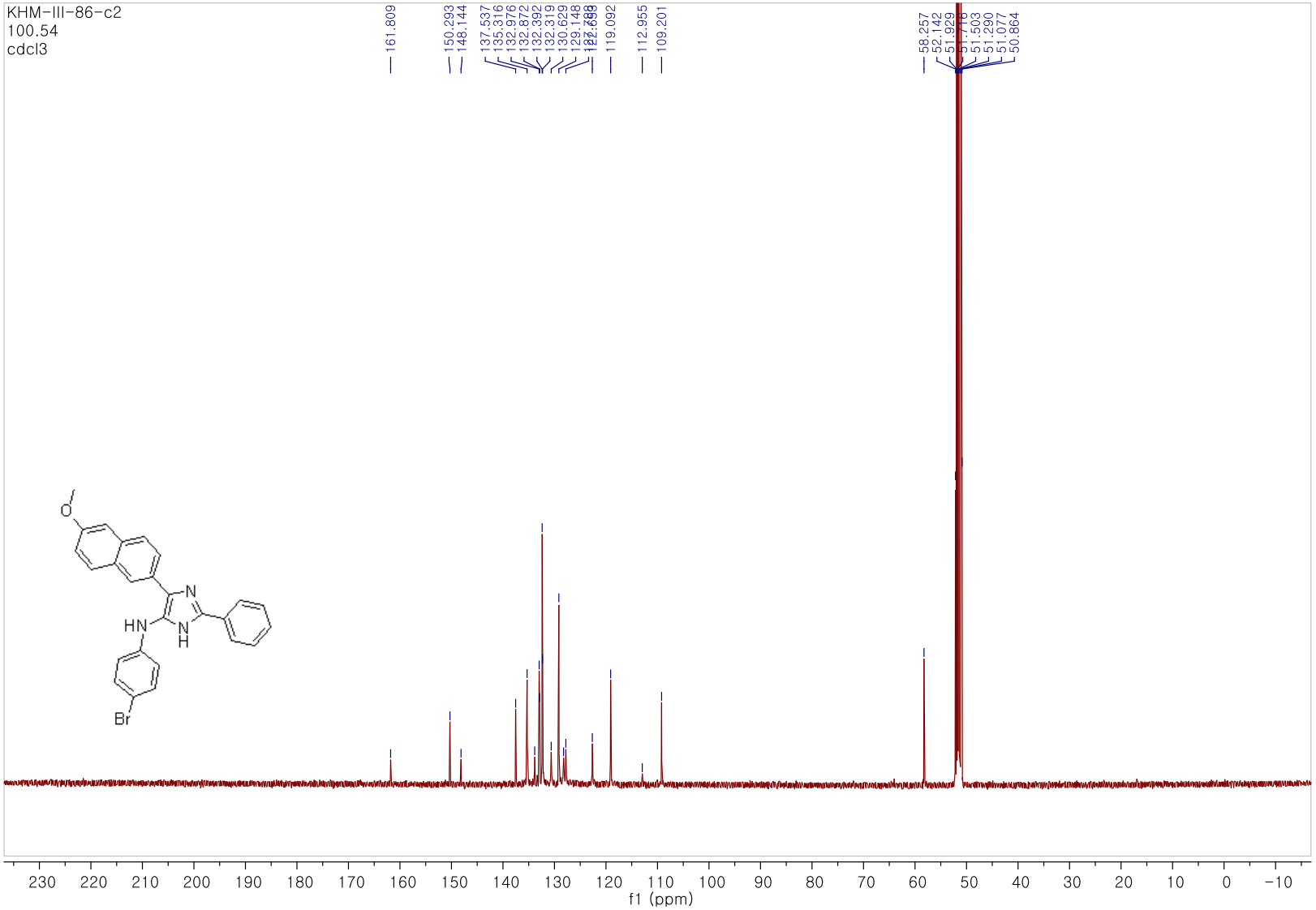
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4af**



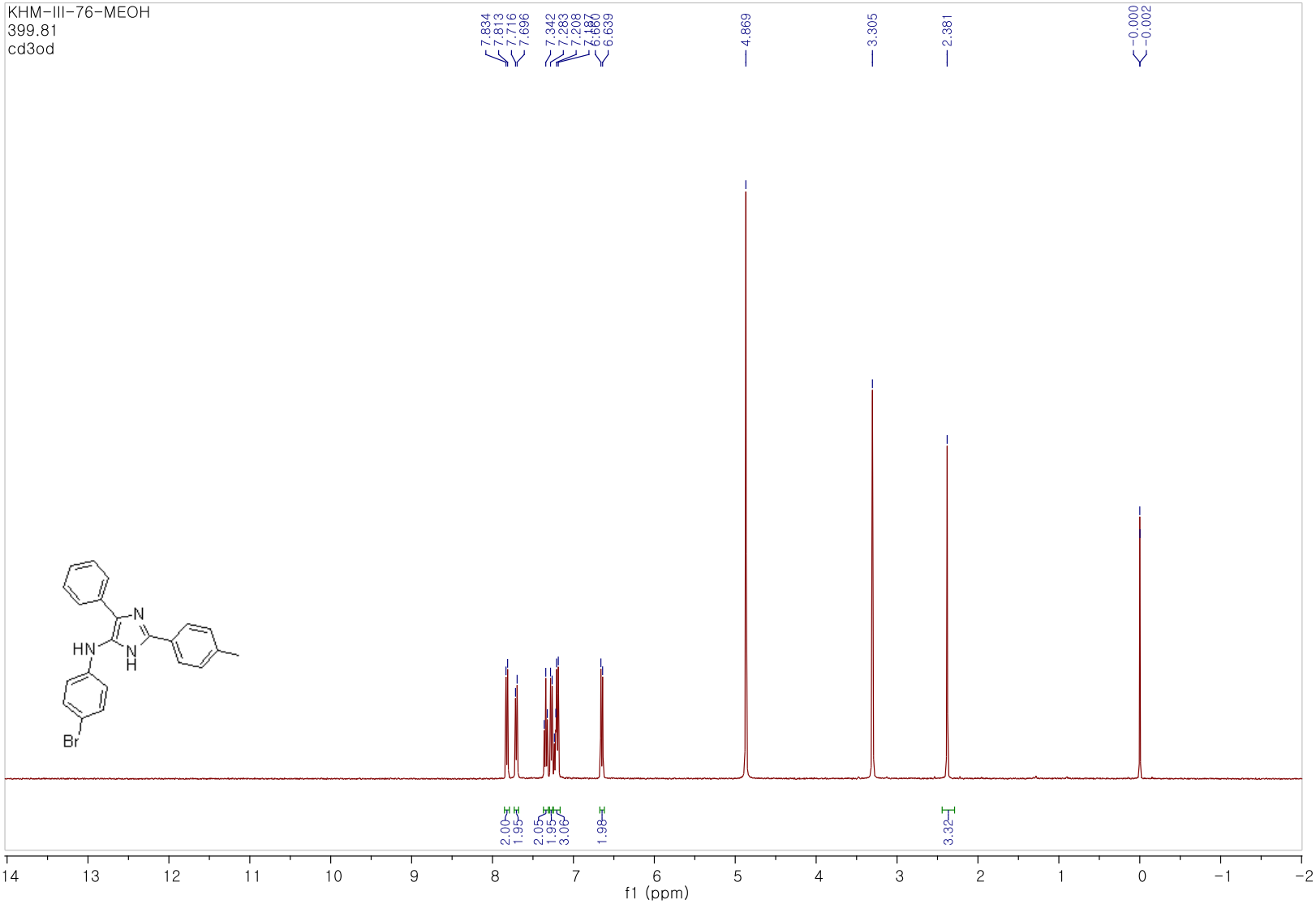
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ag**



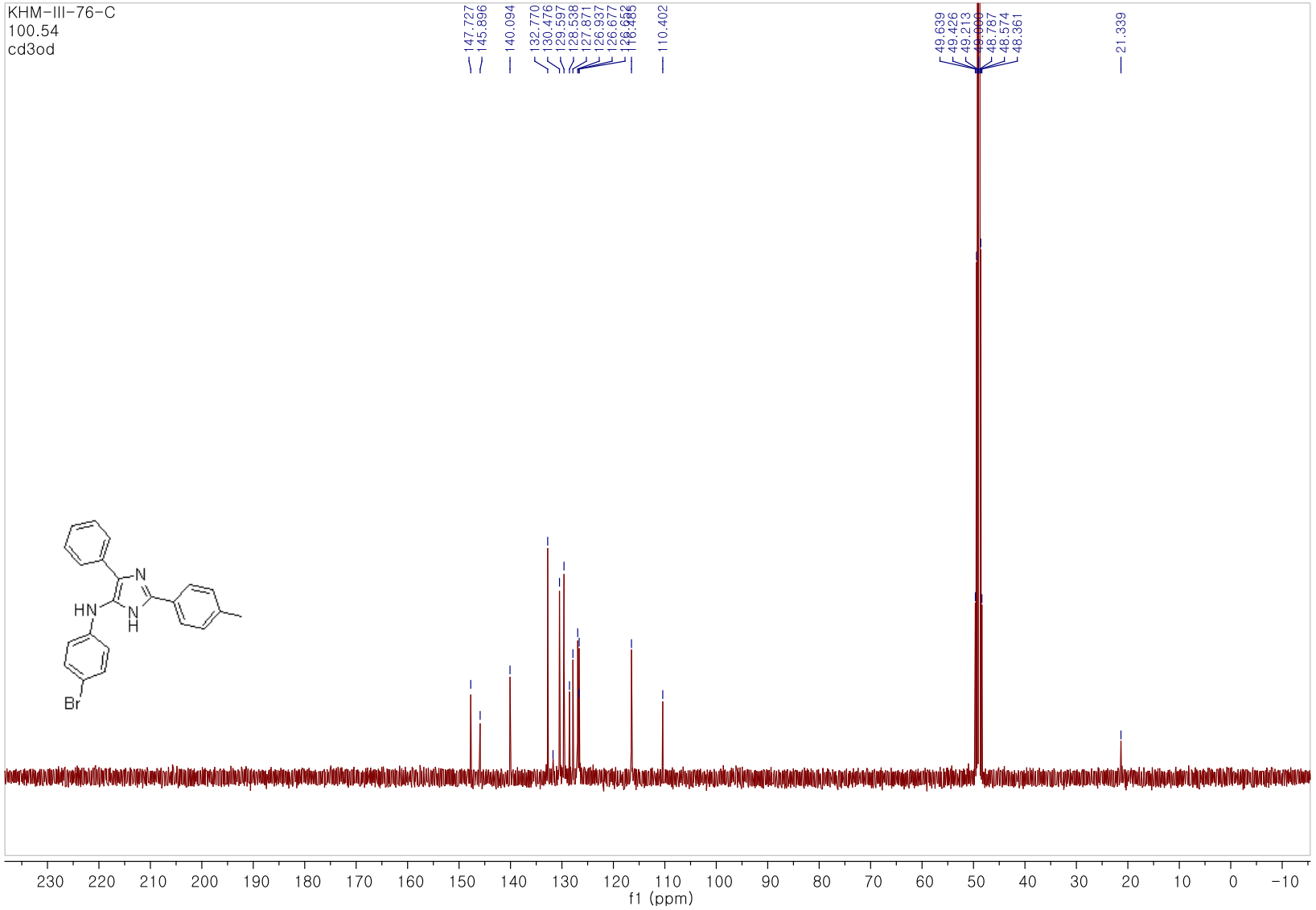
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ag**



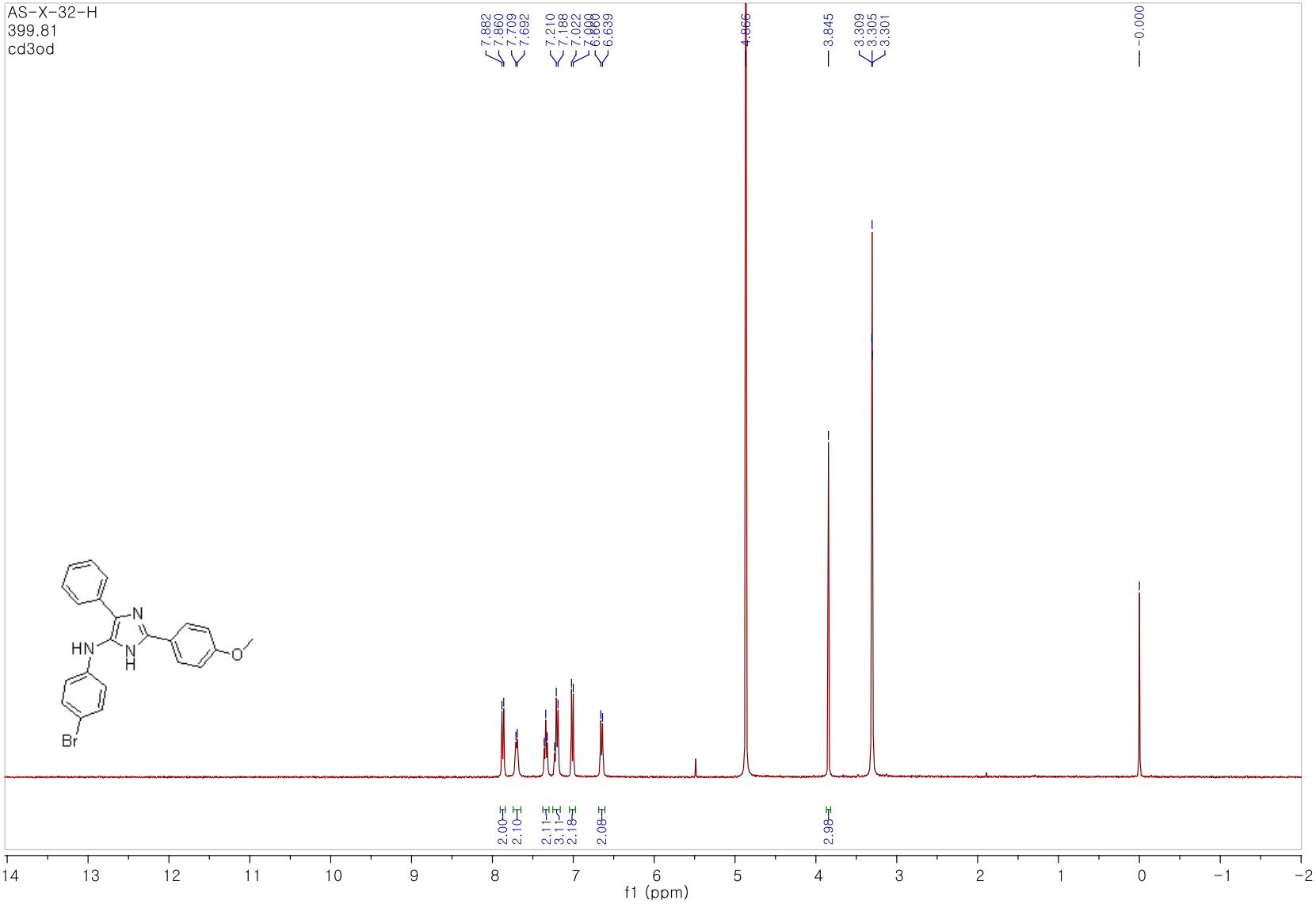
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ah**



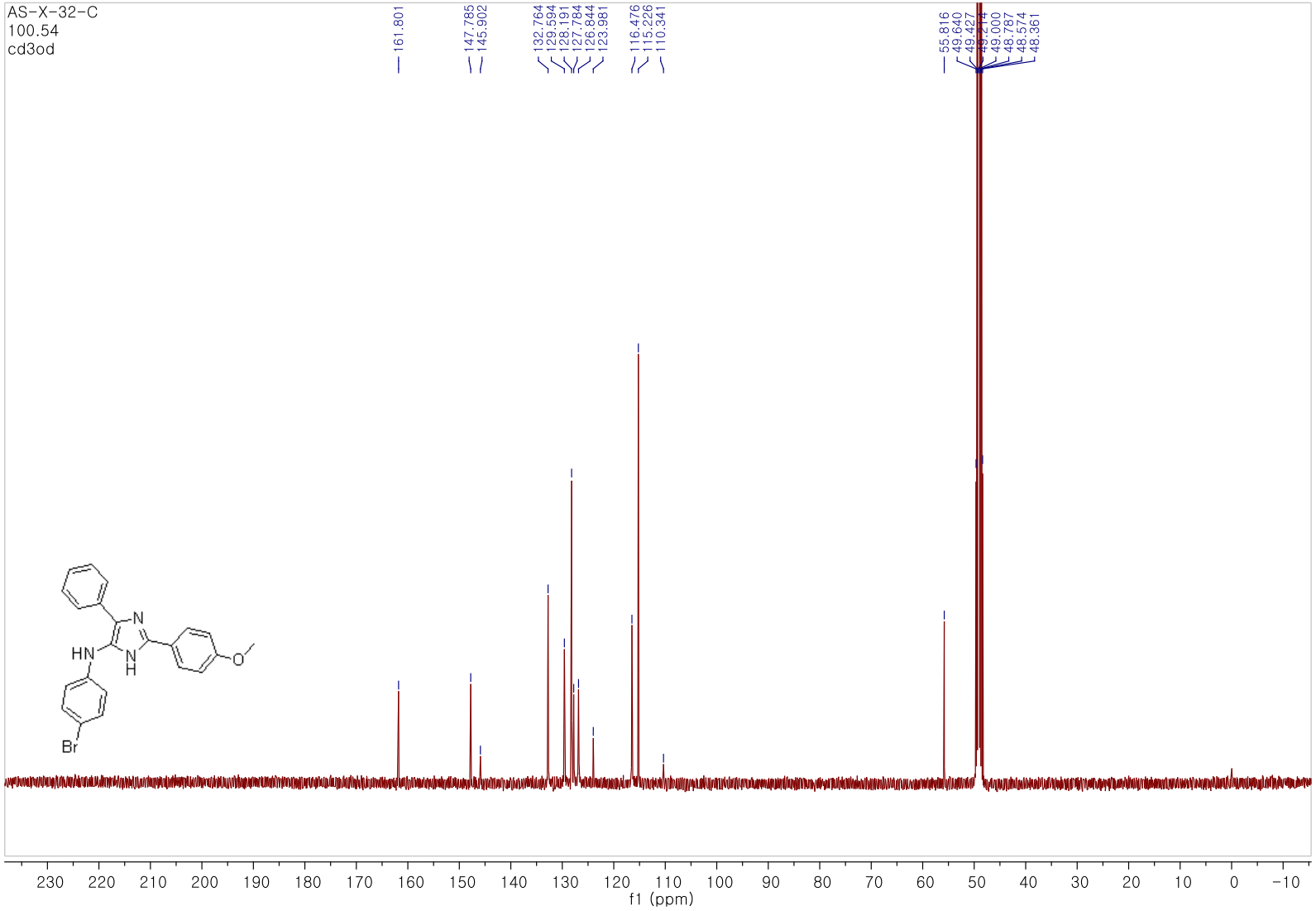
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ah**



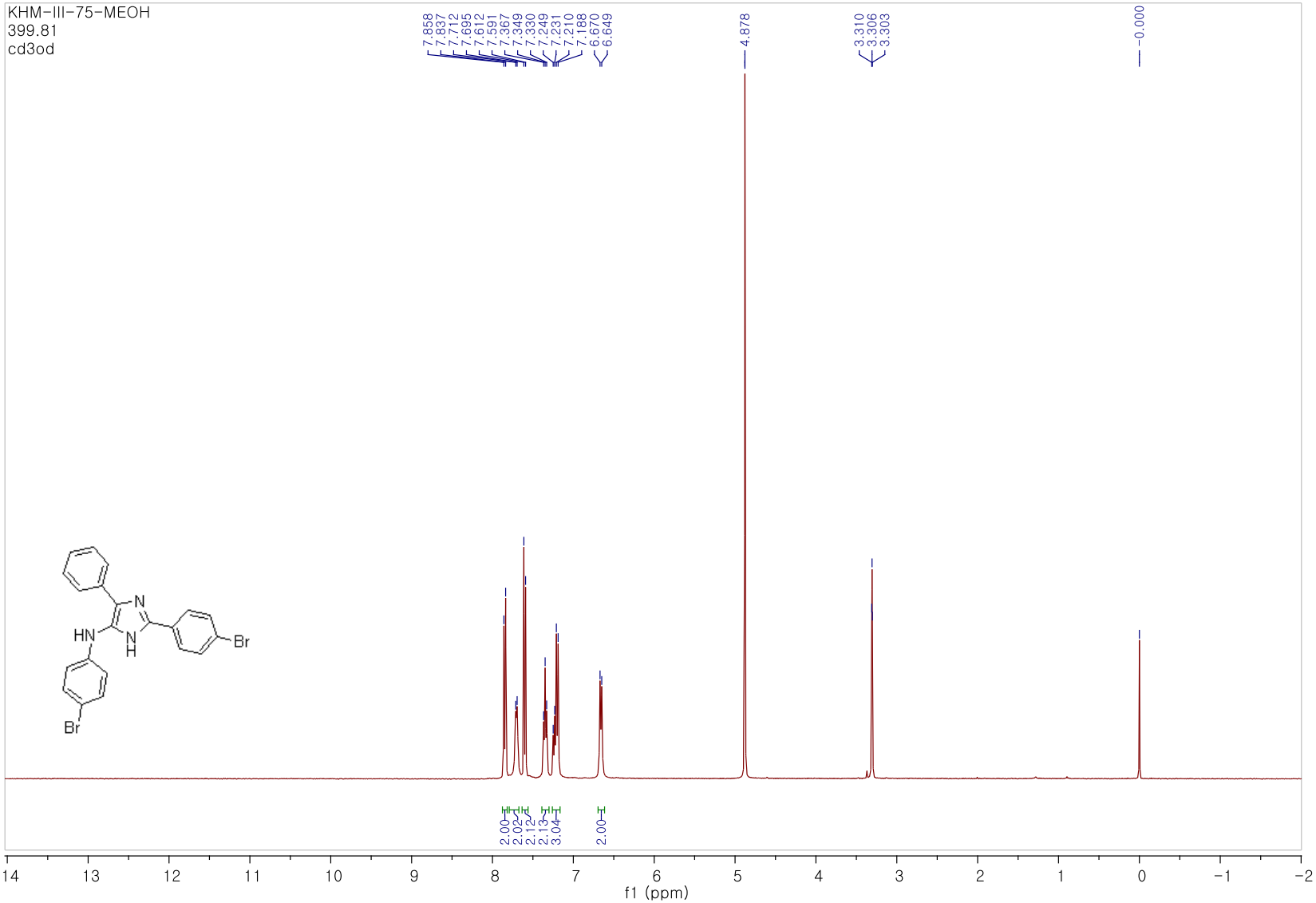
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ai**



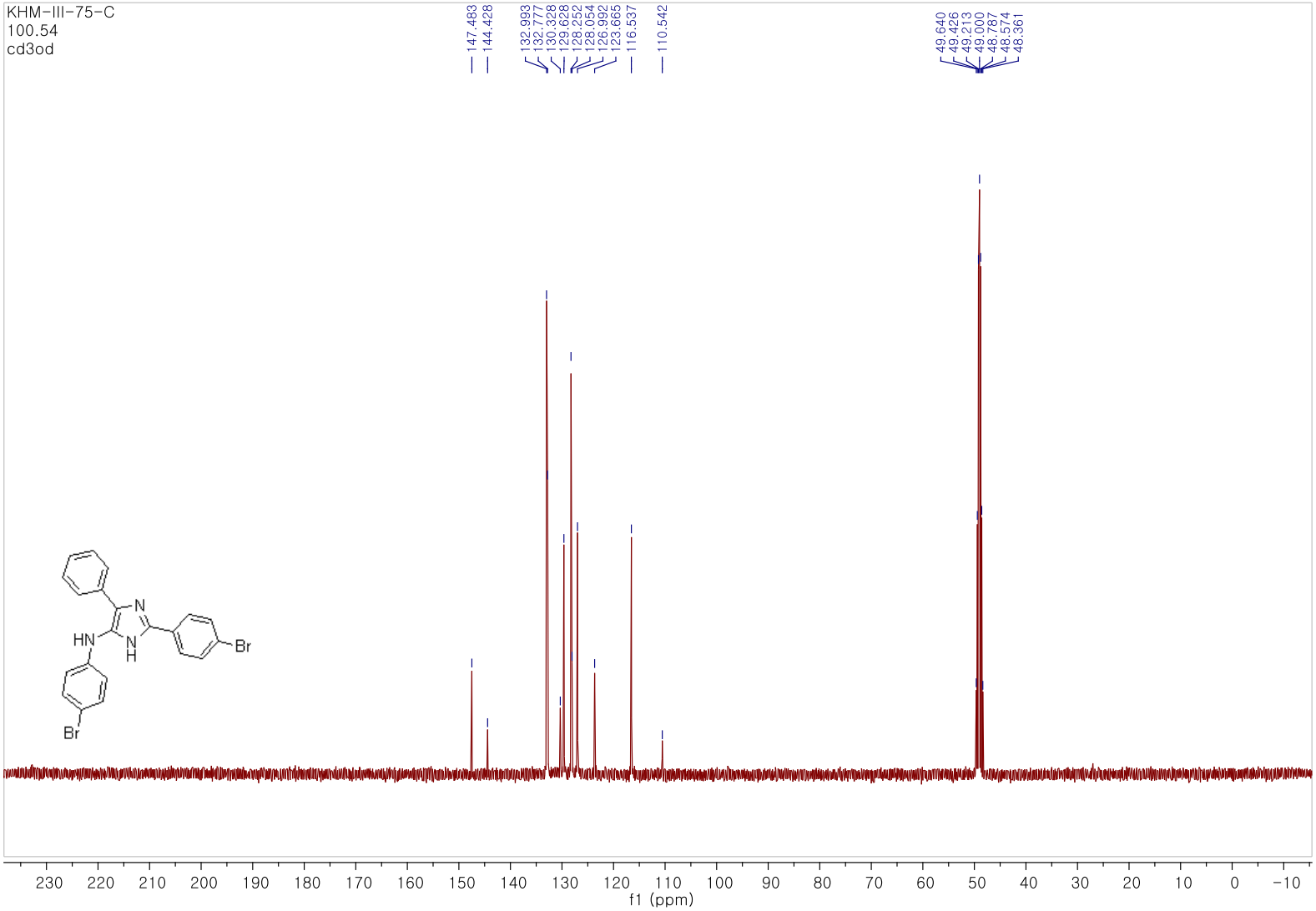
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ai**



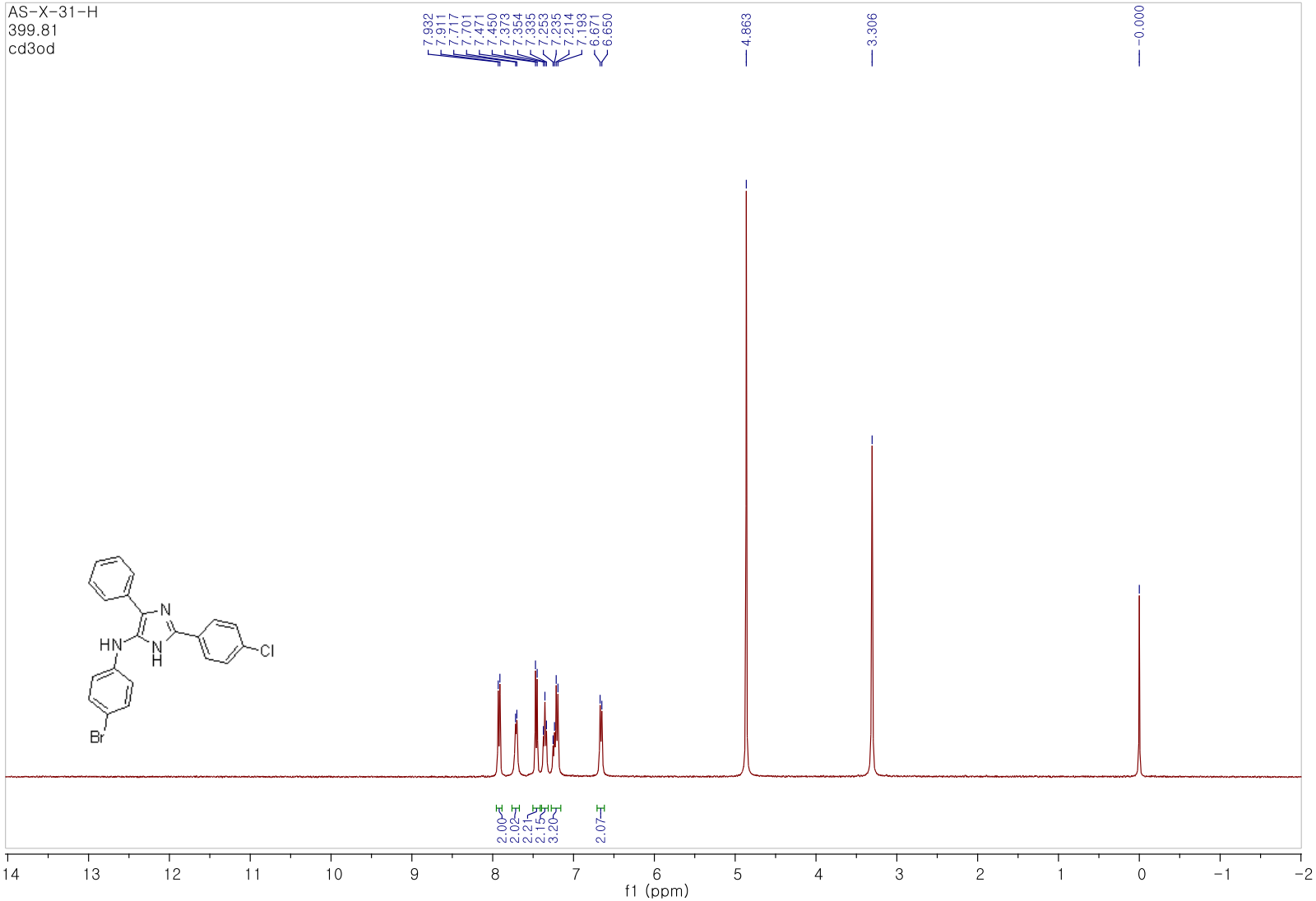
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4aj**



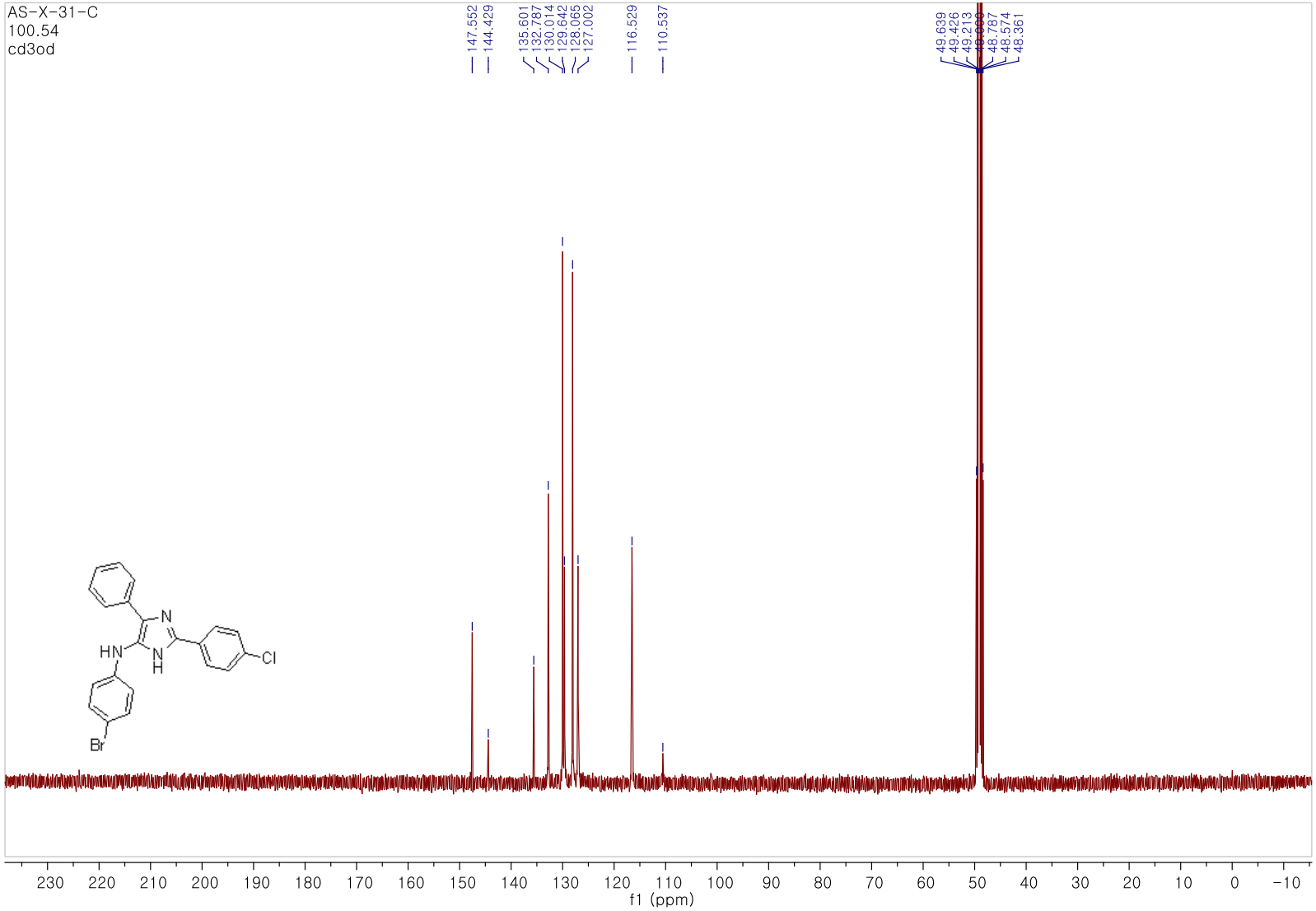
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4aj**



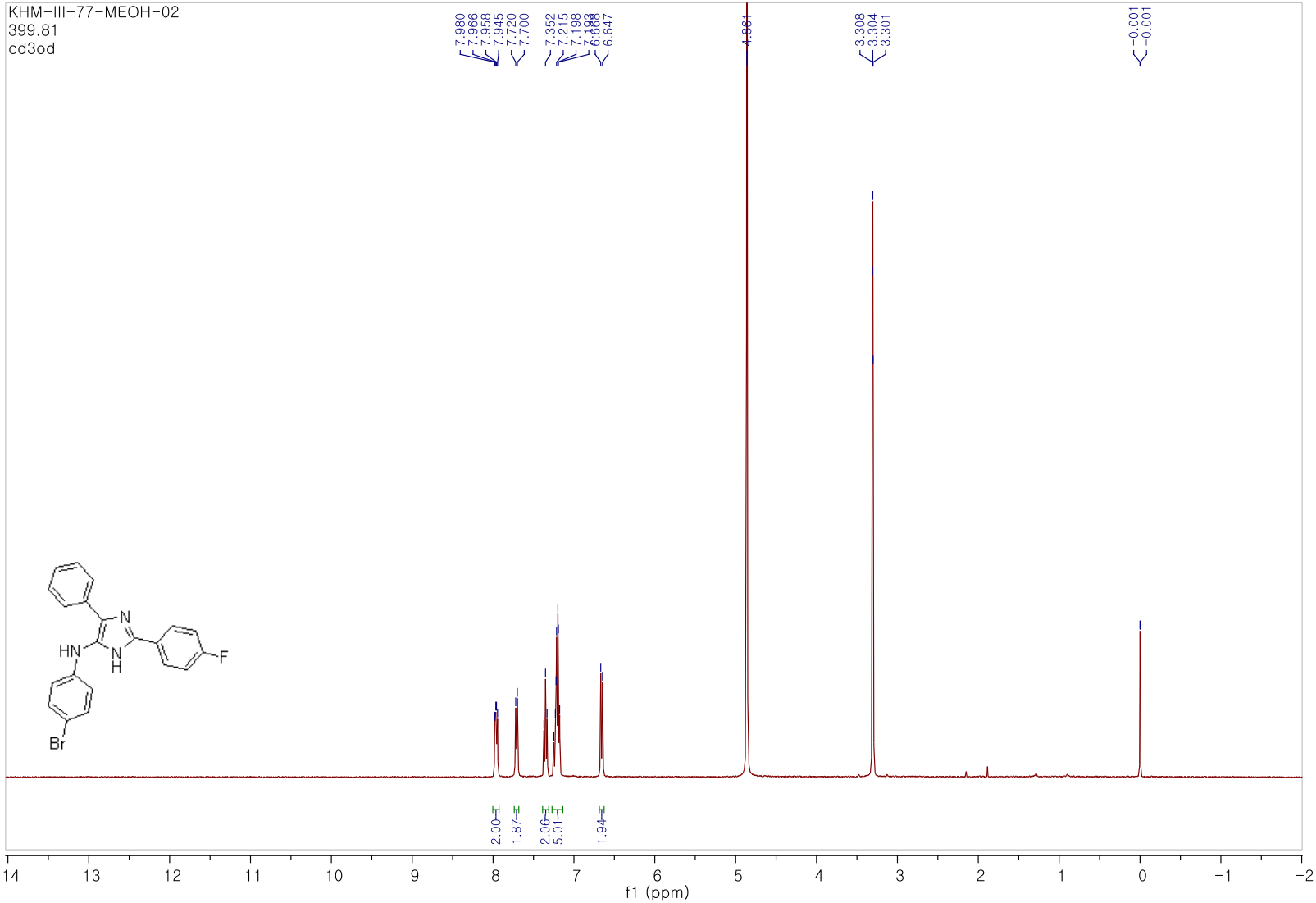
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ak**



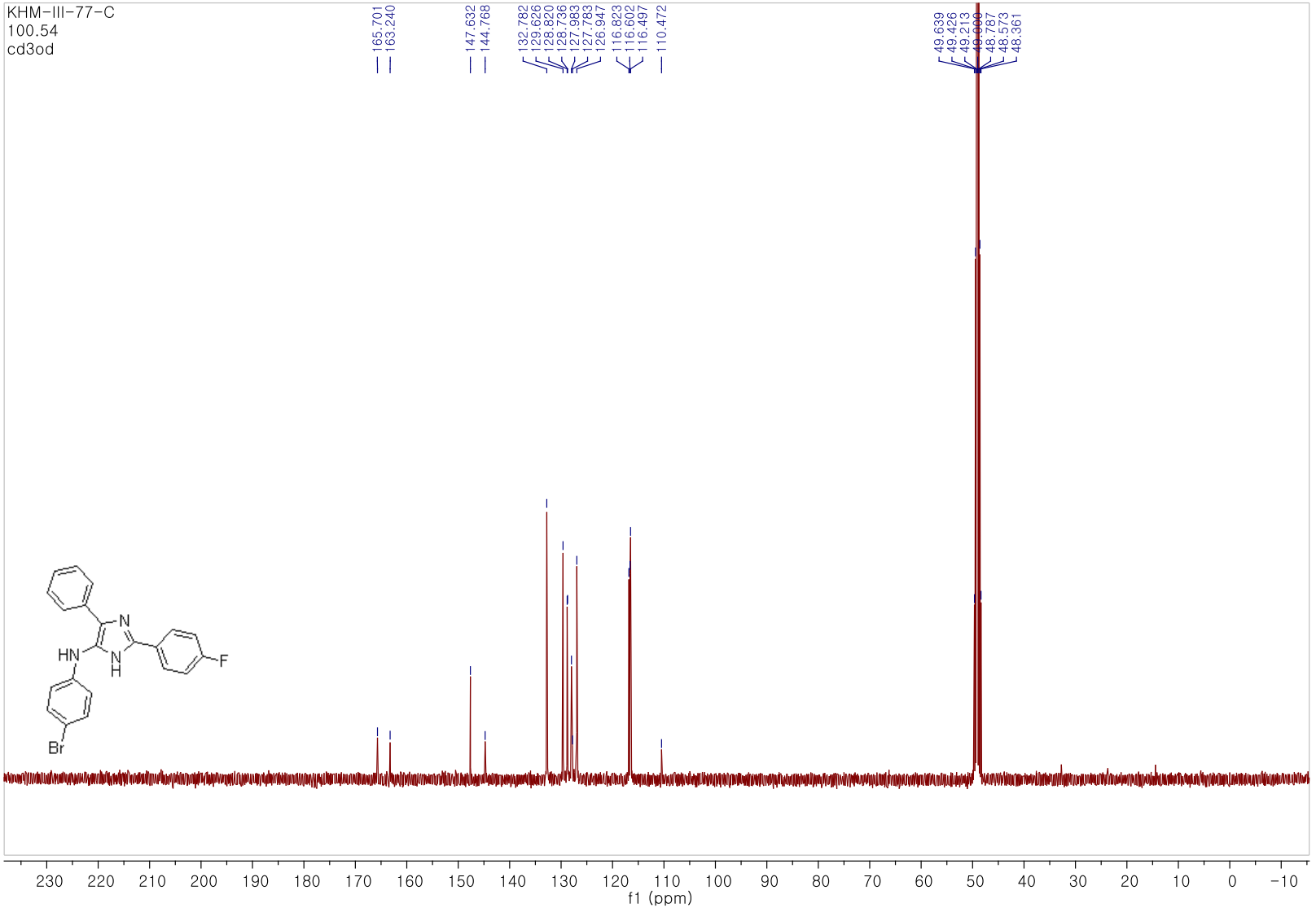
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ak**



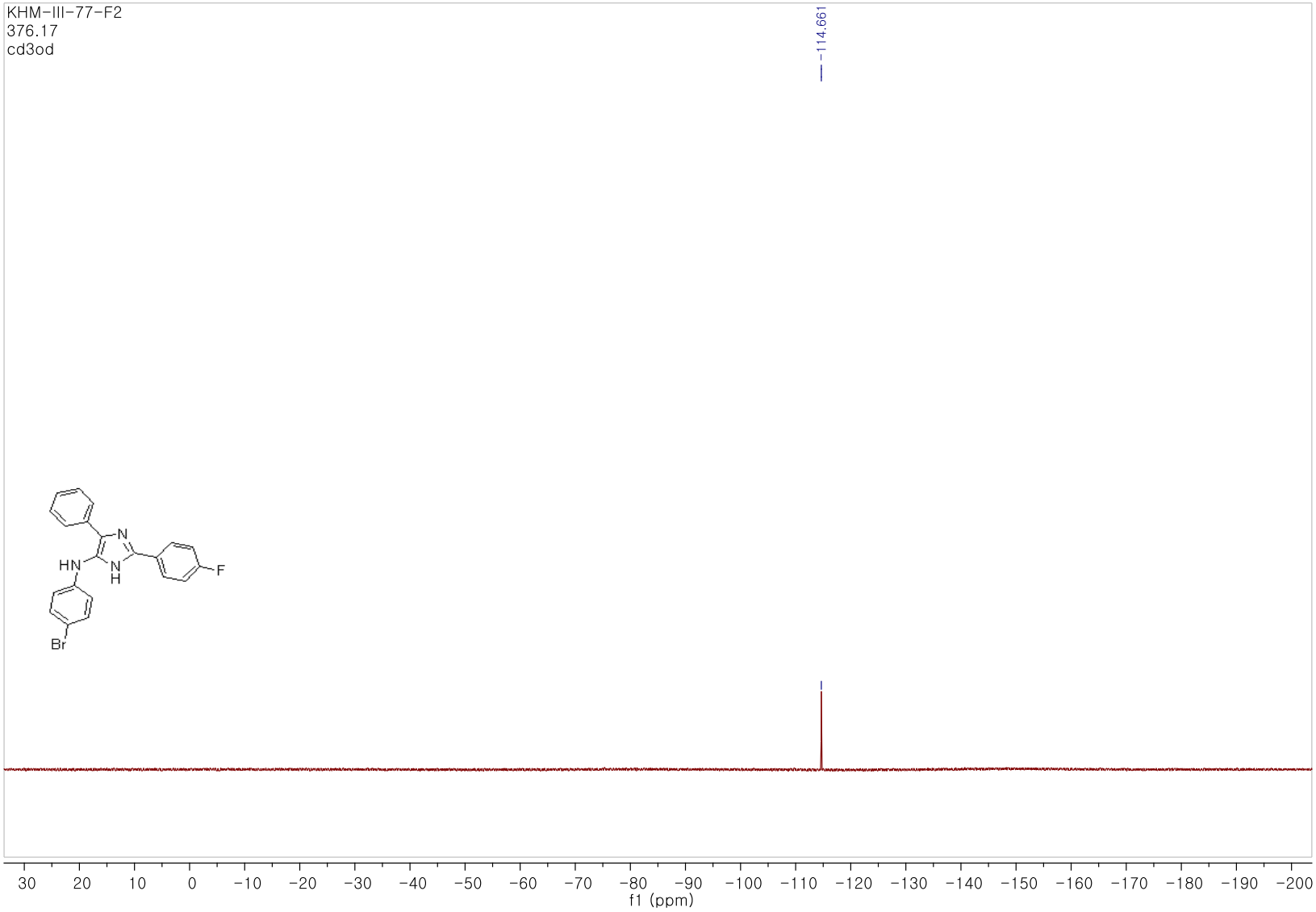
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4al**



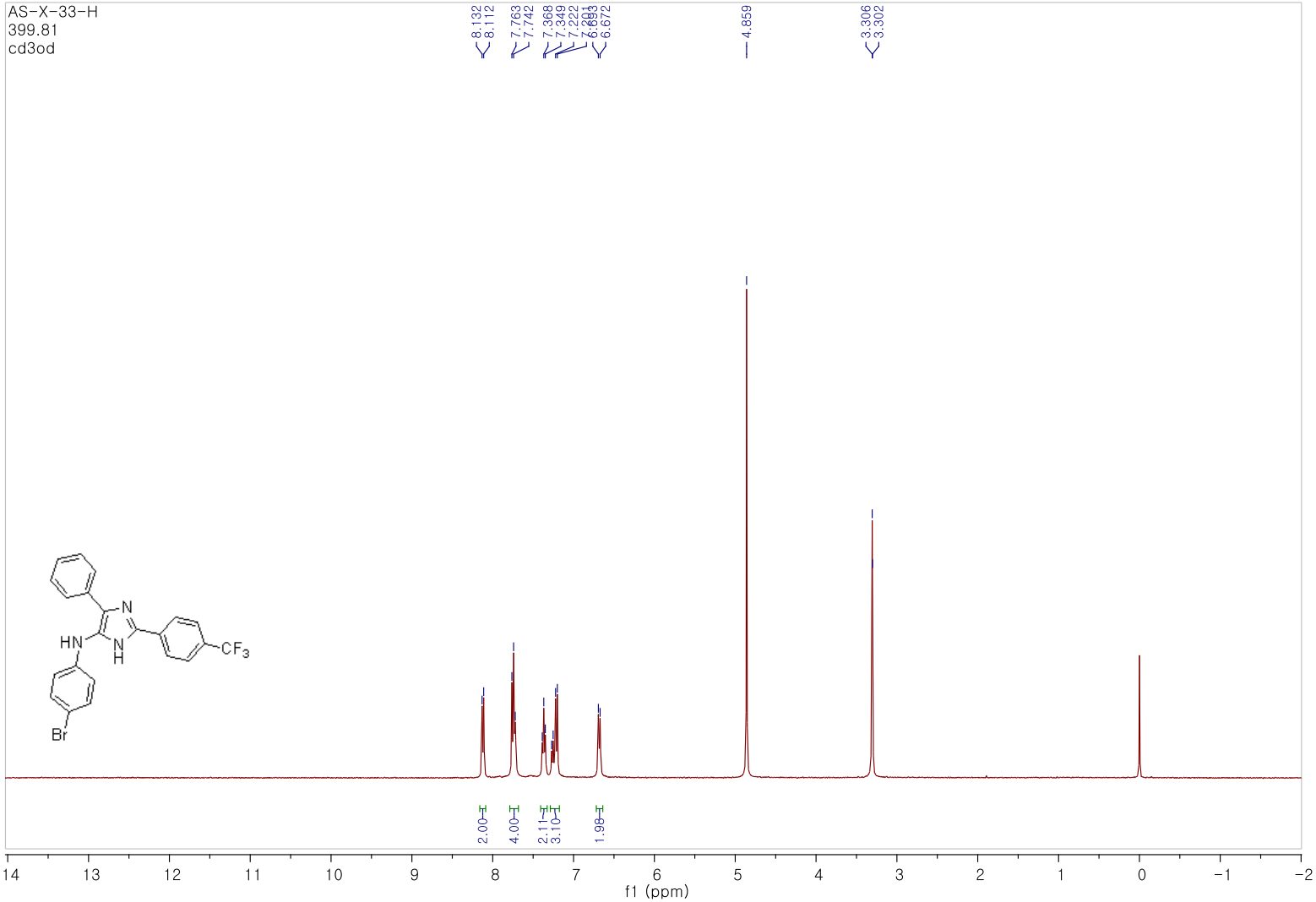
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4al**



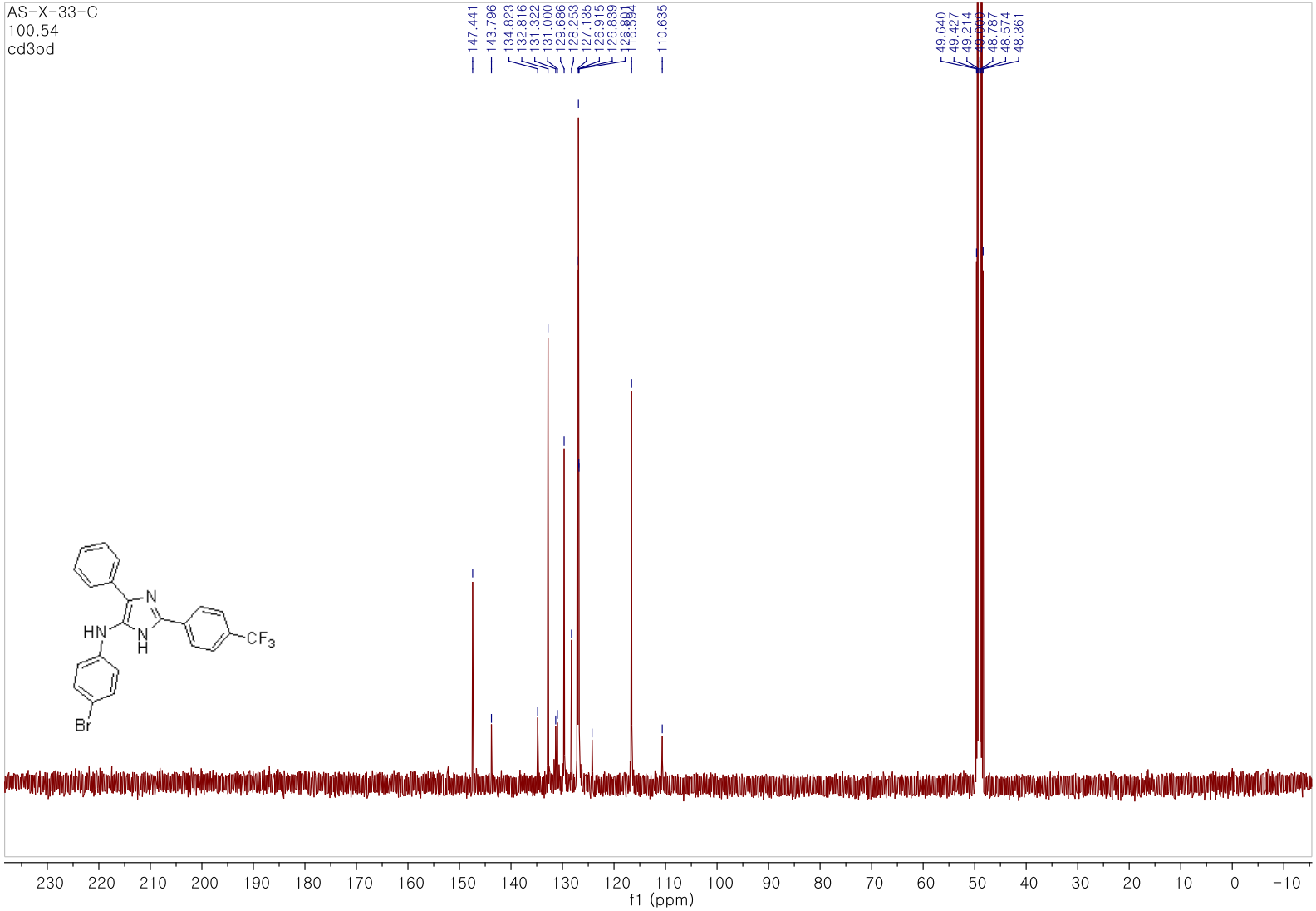
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4al**



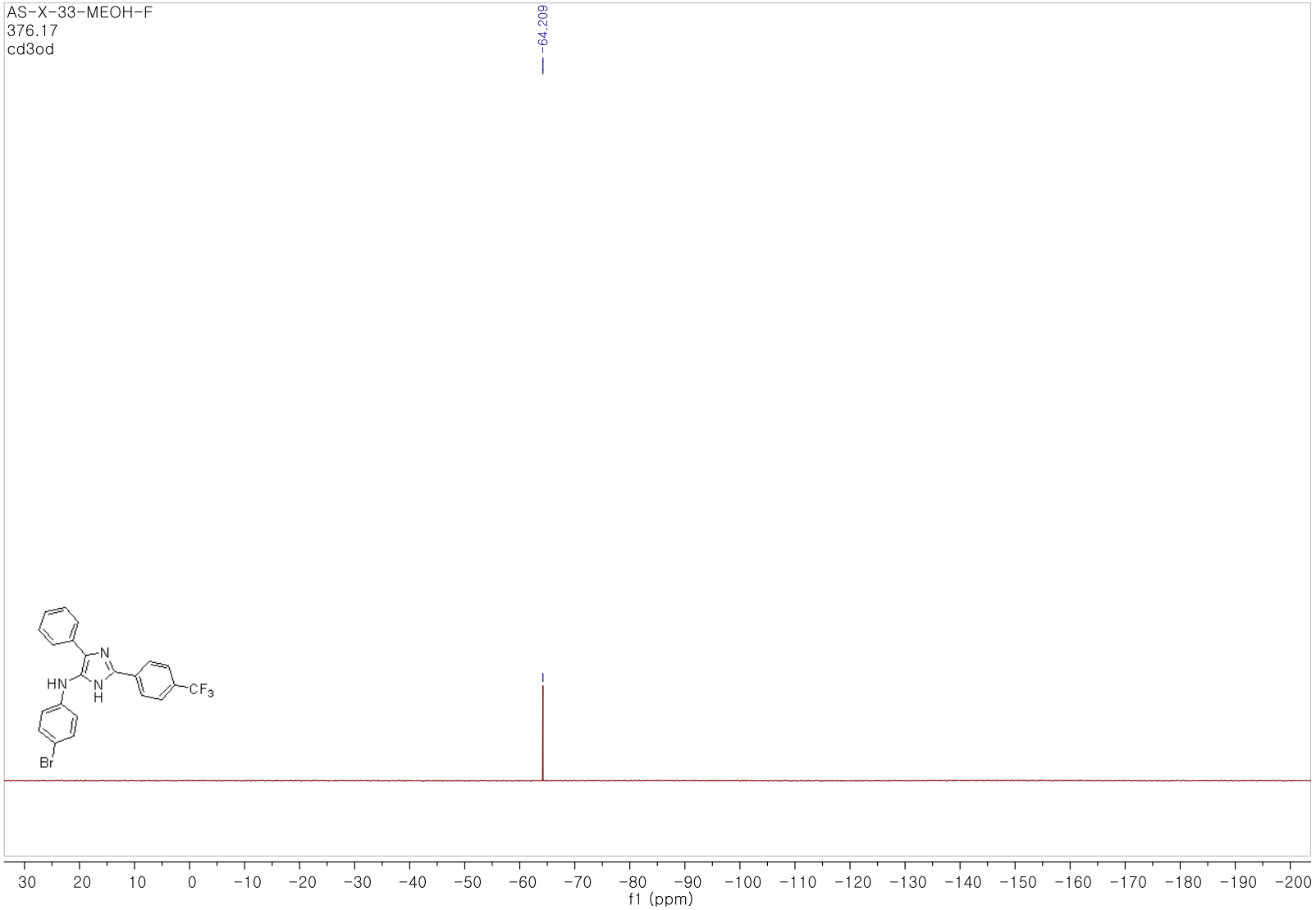
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4am**



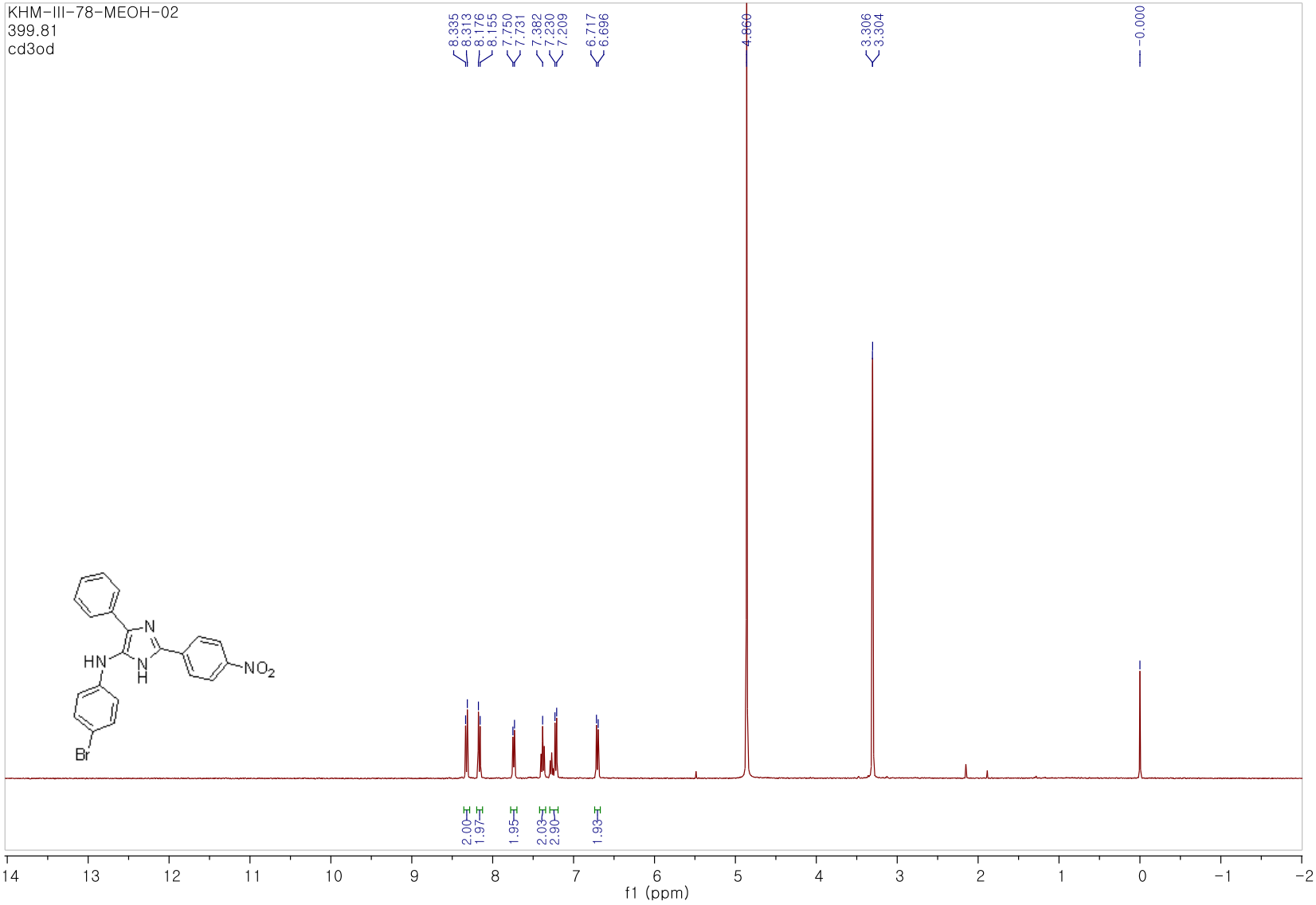
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4am**



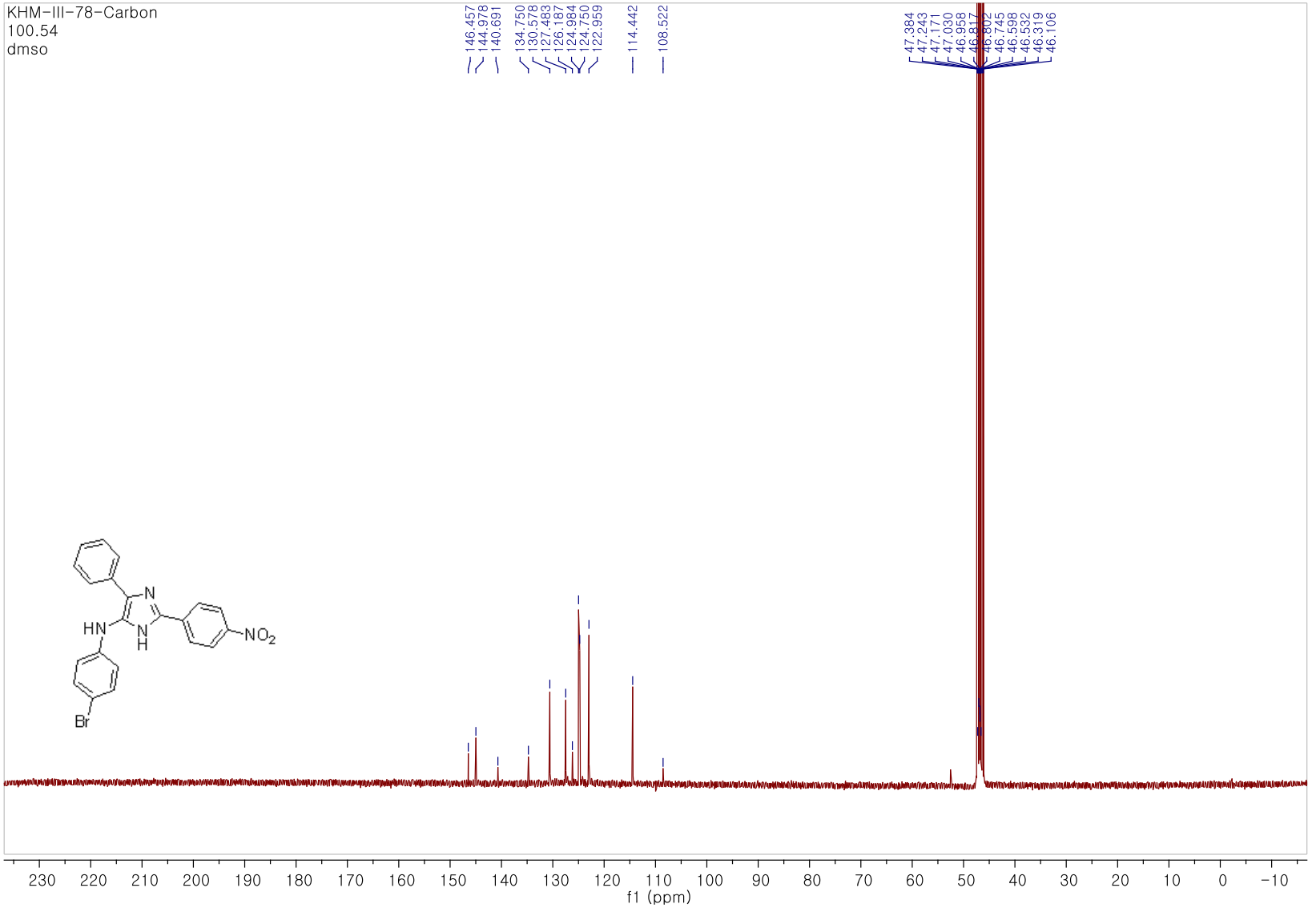
^{19}F NMR (376 MHz, methanol-d_4) spectrum of **4am**



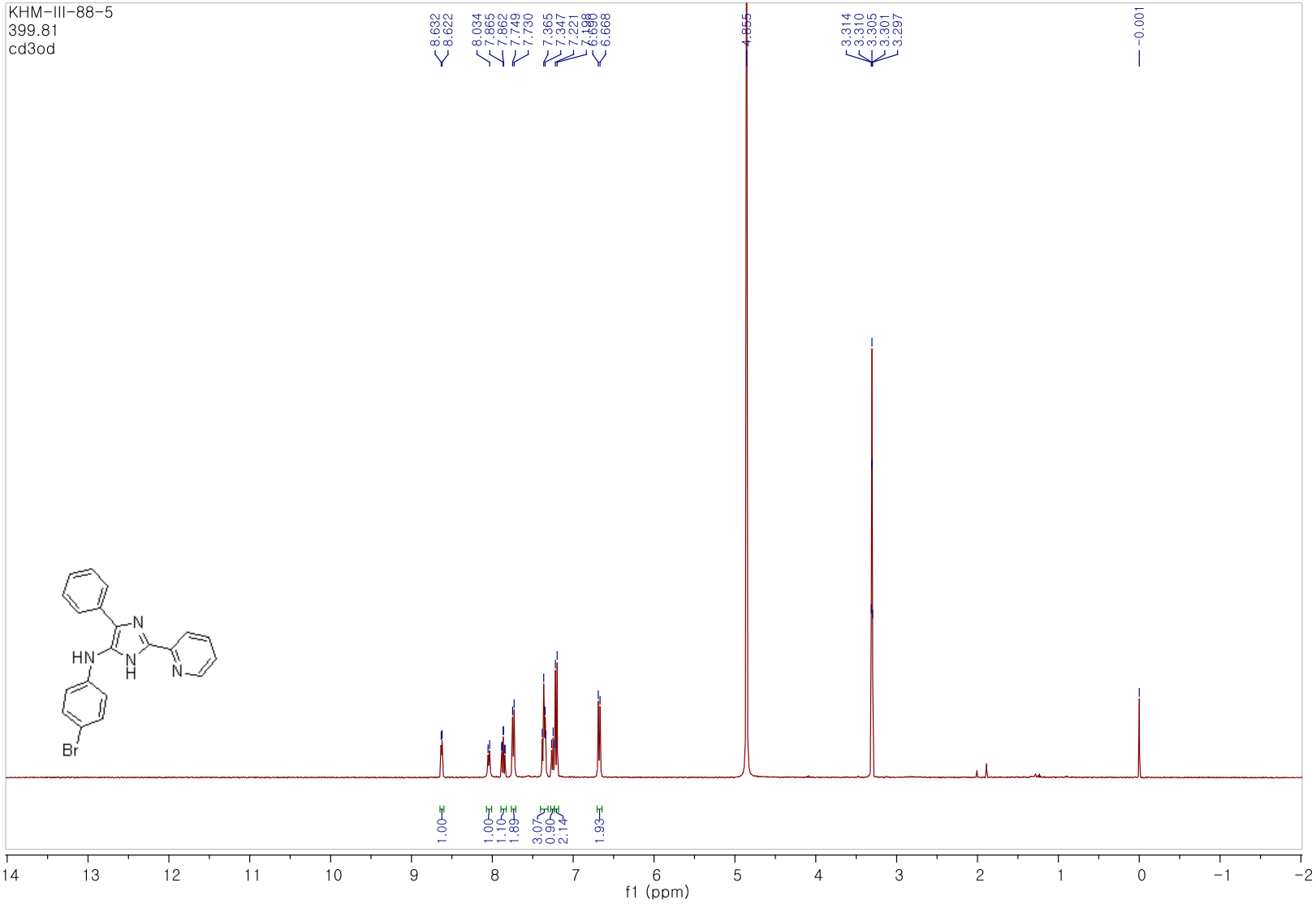
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4an**



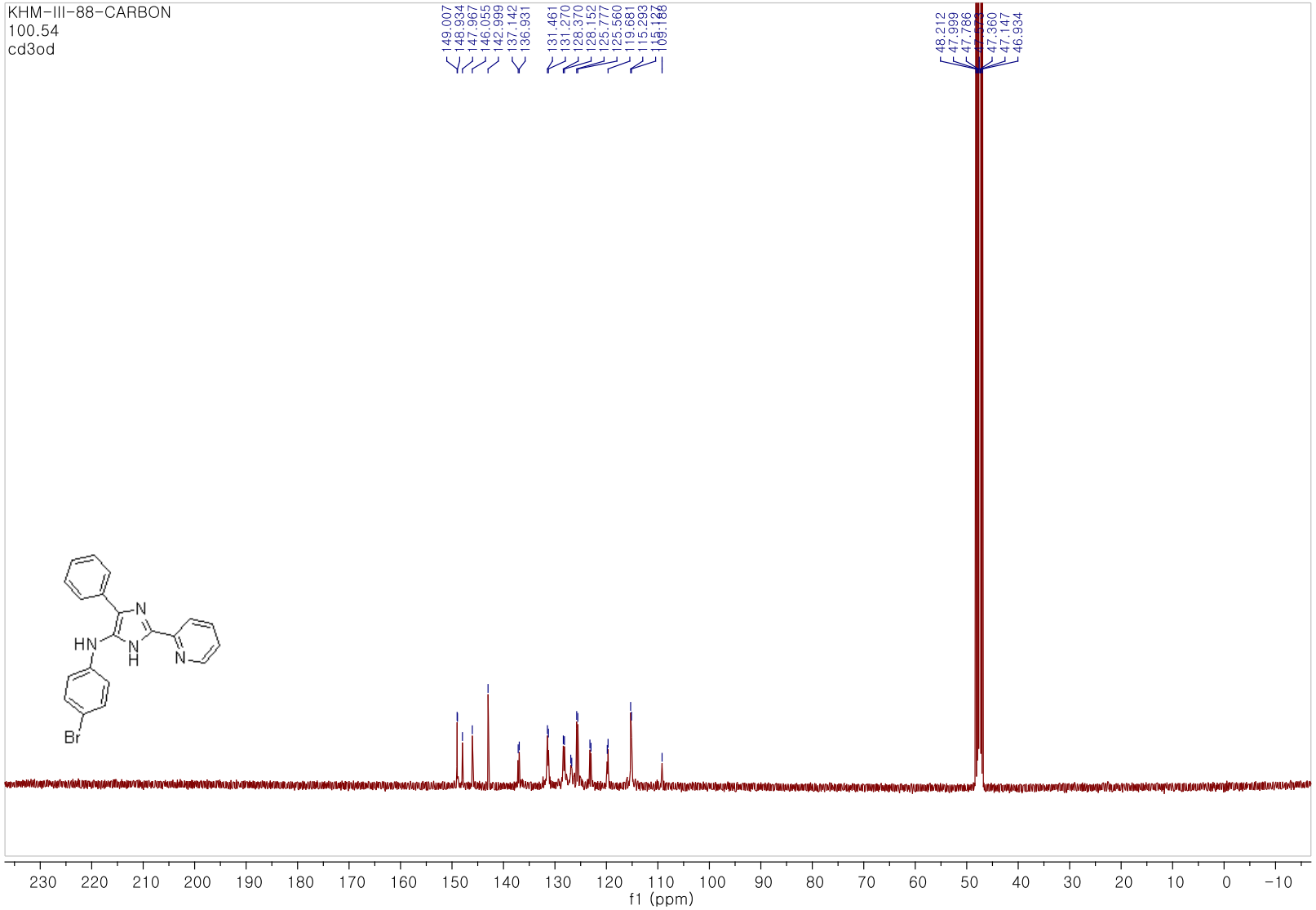
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4an**



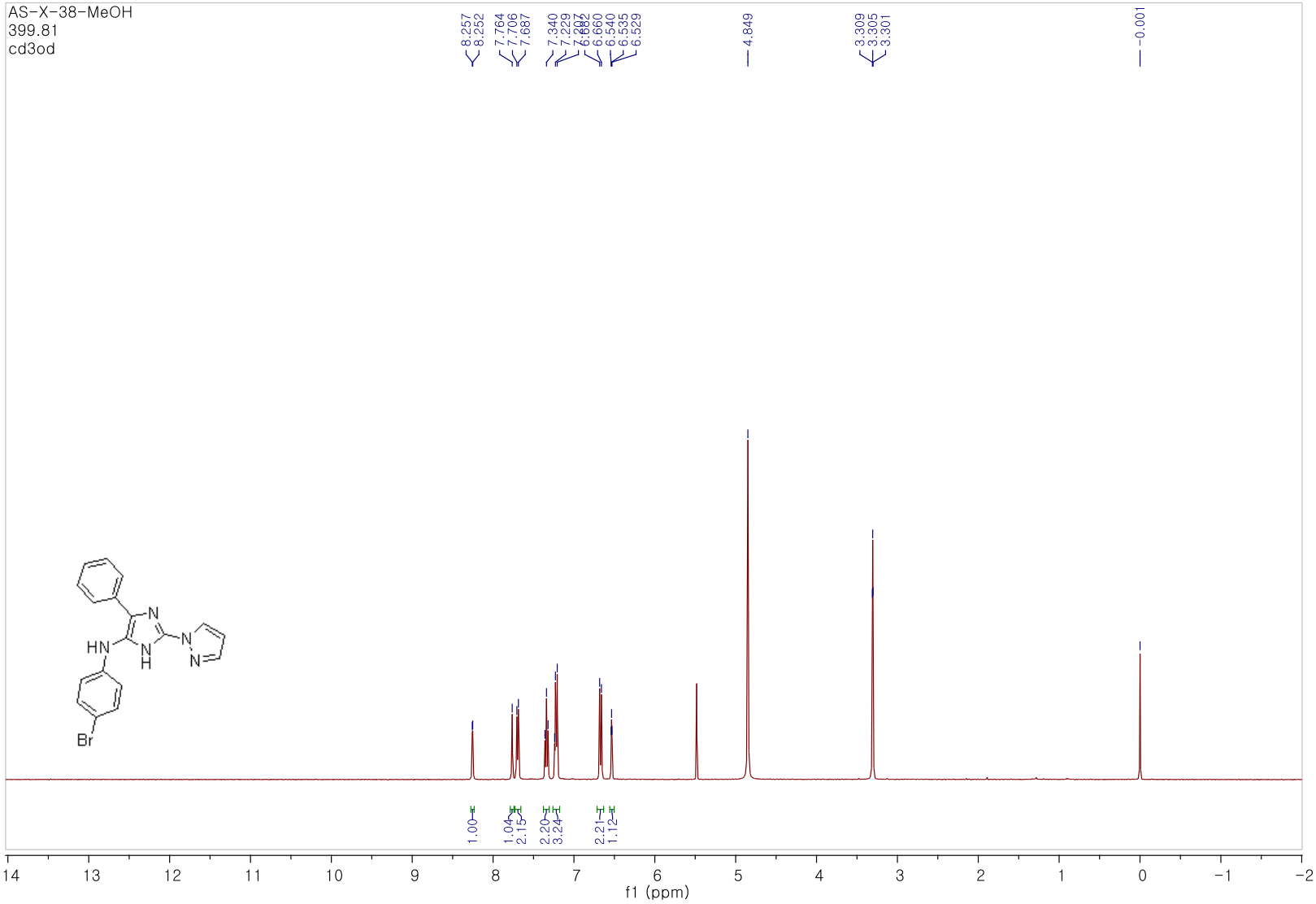
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ao**



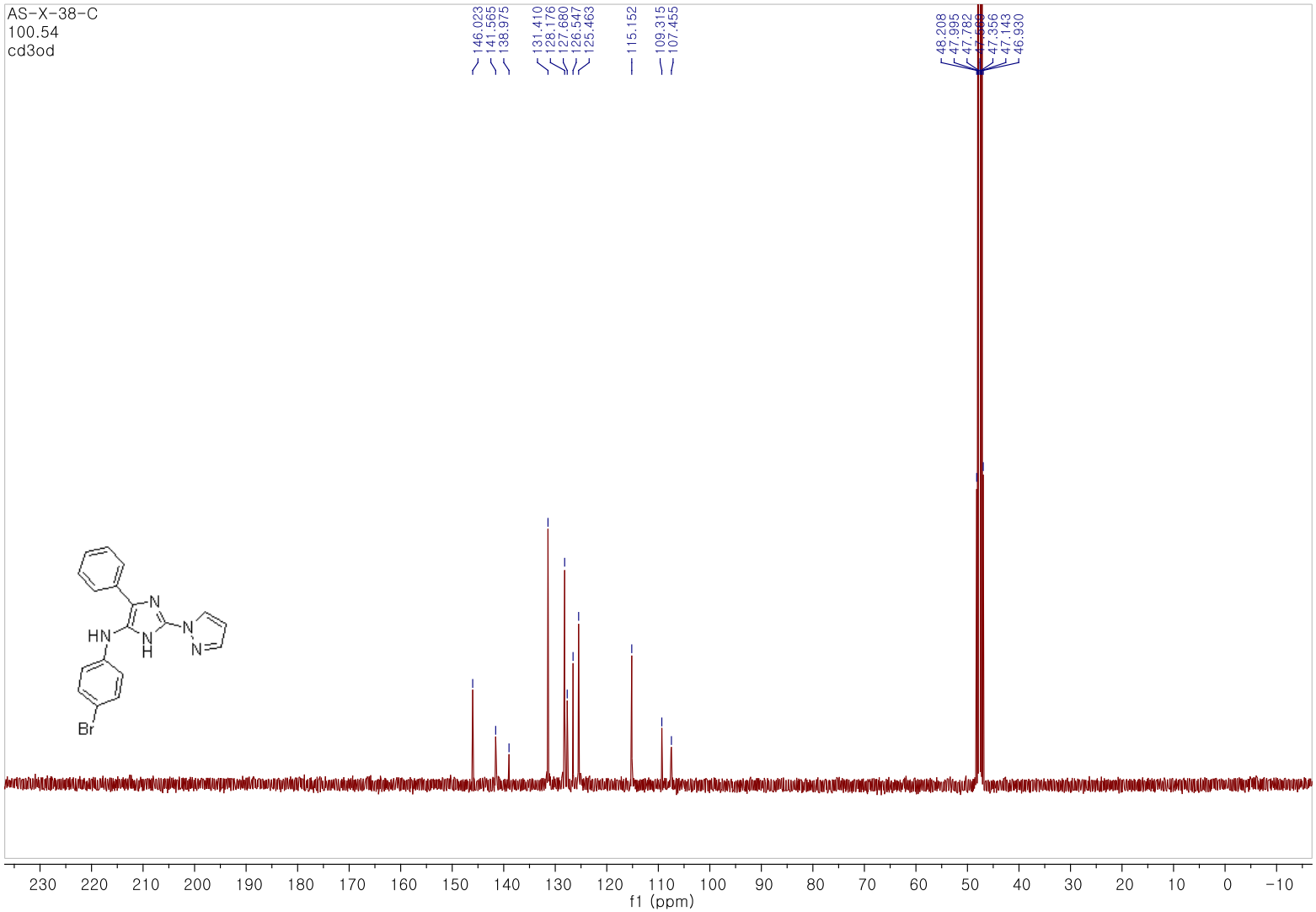
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ao**



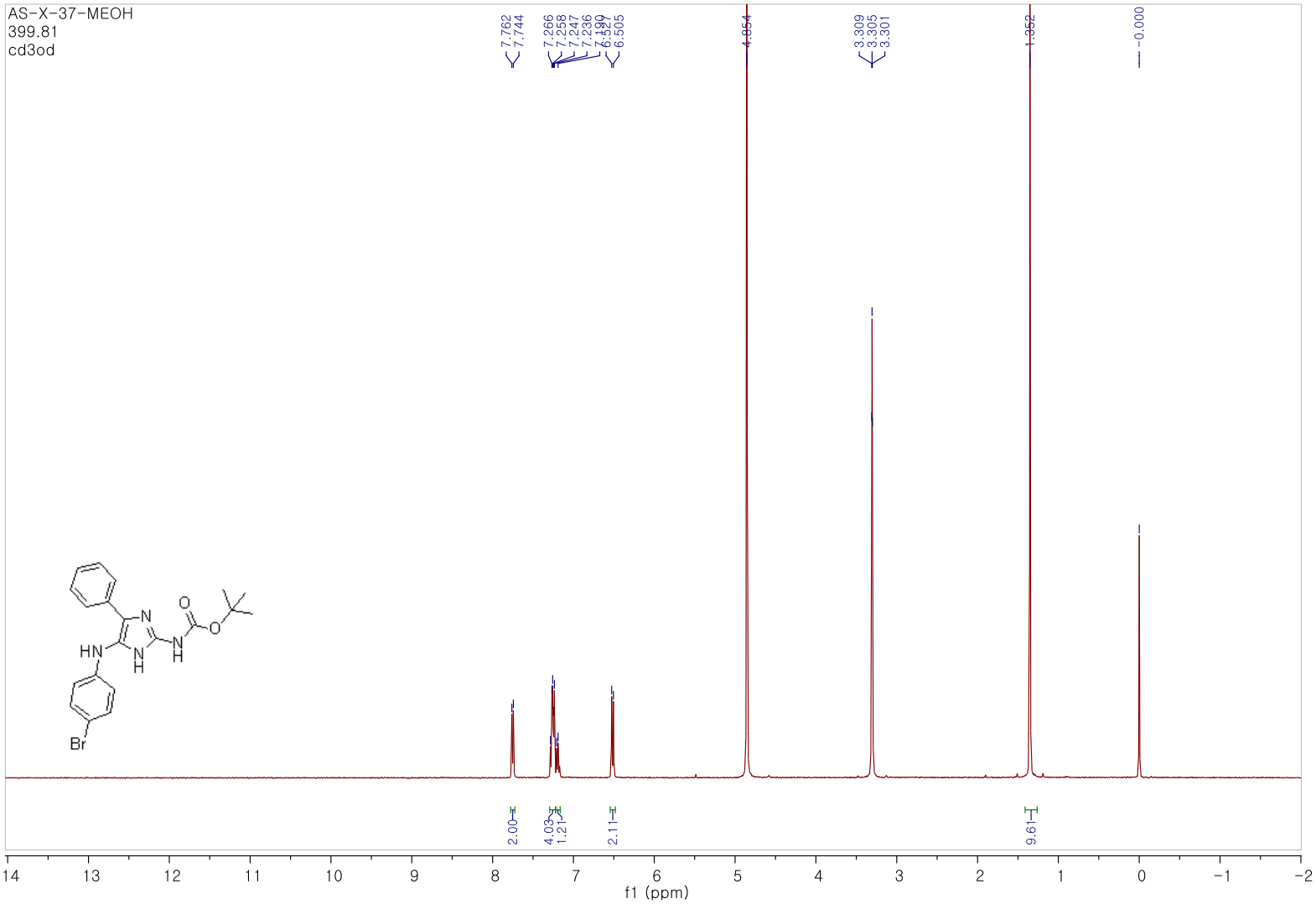
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4ap**



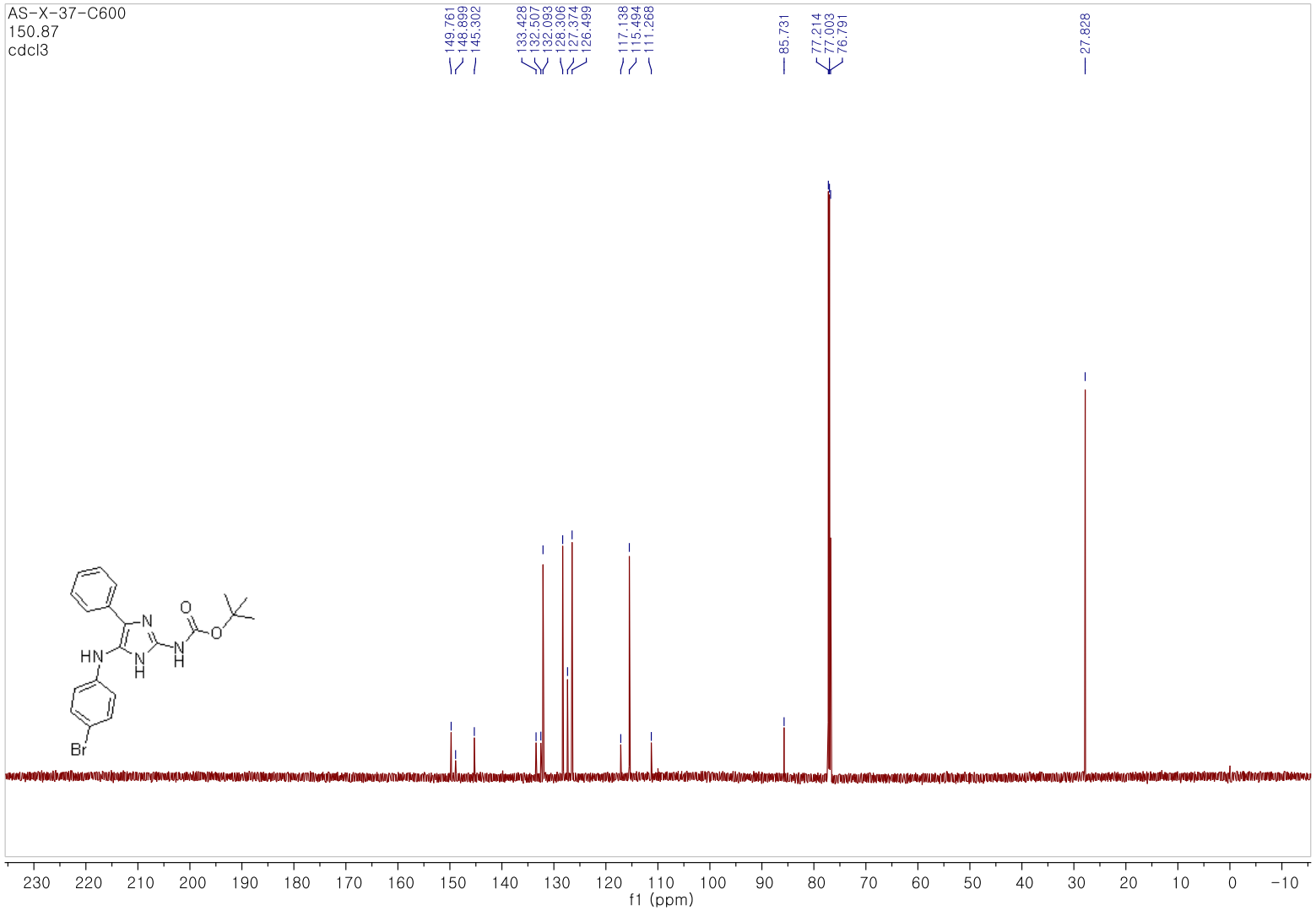
^{13}C NMR (100 MHz, methanol-d_4) spectrum of **4ap**



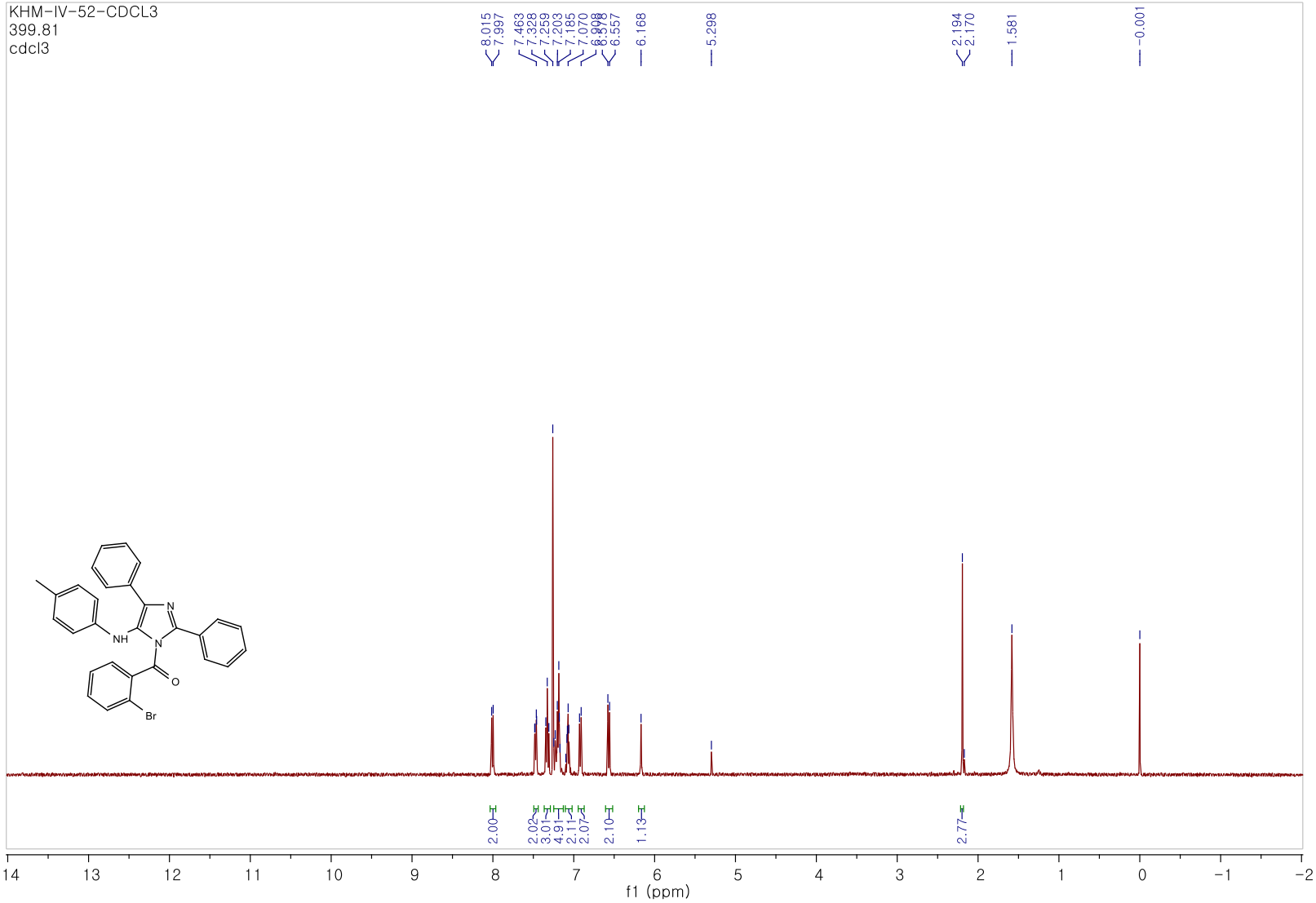
^{1}H NMR (400 MHz, methanol-d_4) spectrum of **4aq**



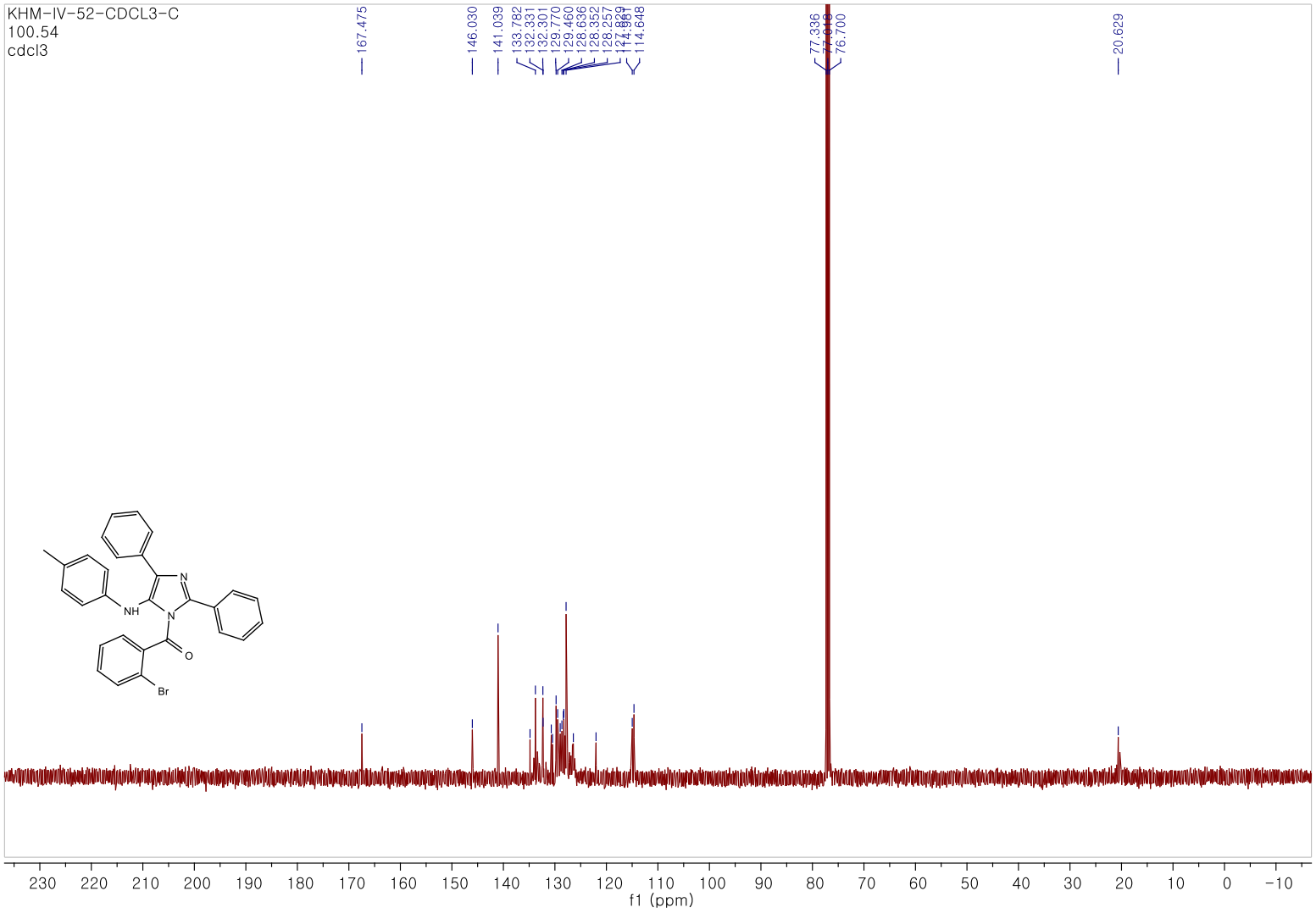
^{13}C NMR (100 MHz, methanol -d_4) spectrum of **4aq**



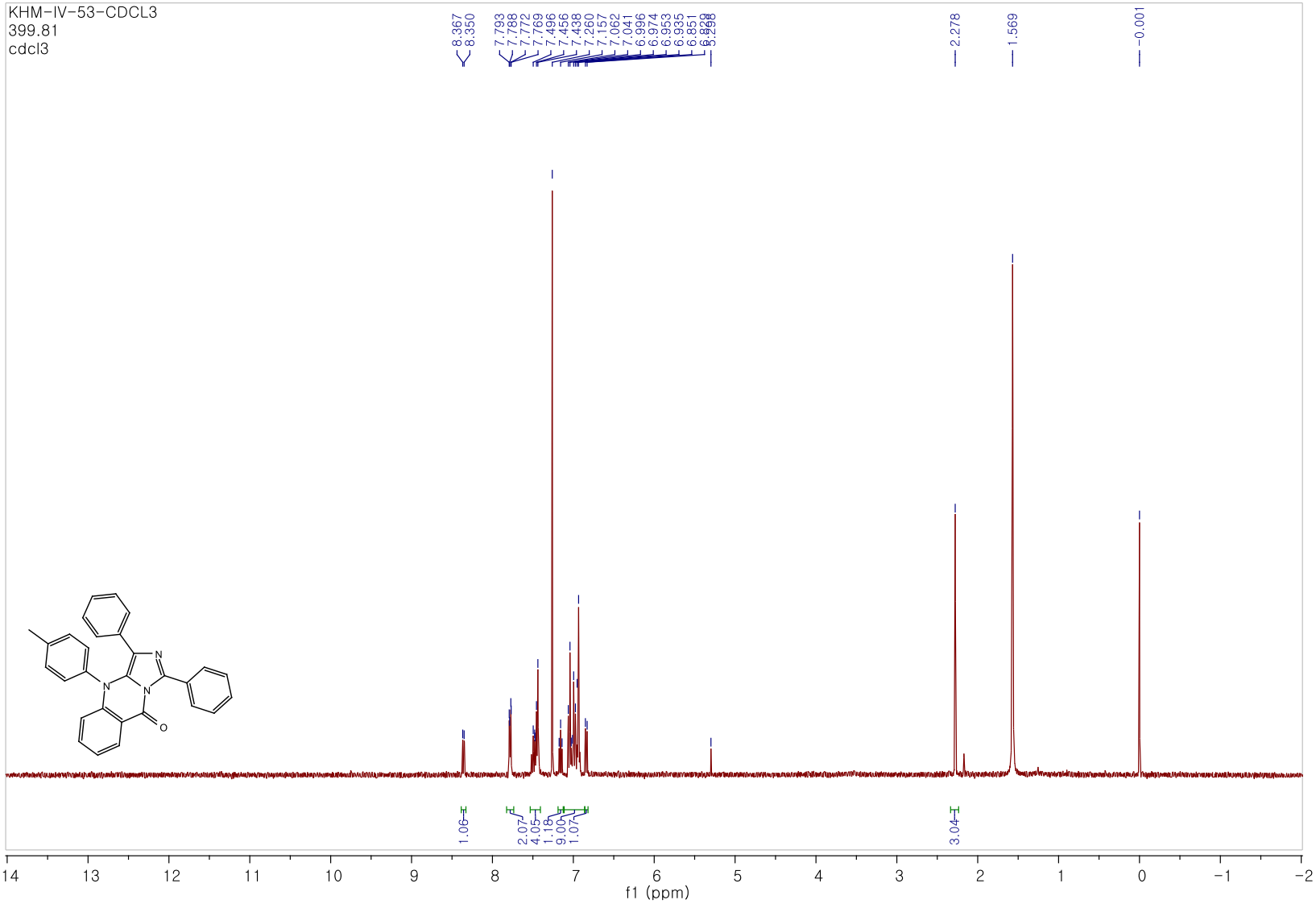
^{1}H NMR (400 MHz, CDCl3) spectrum of **5a**



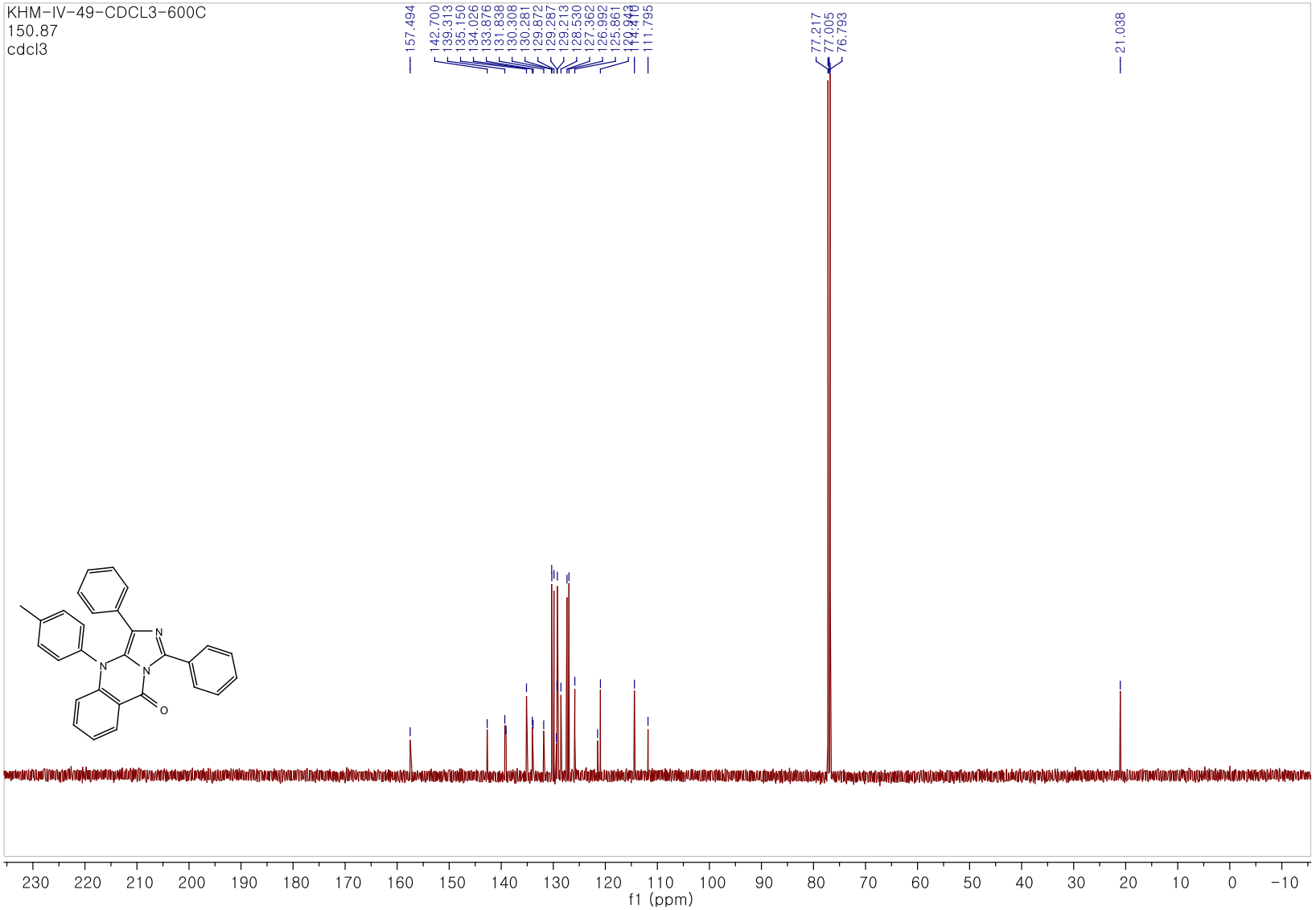
^{13}C NMR (100 MHz, CDCl3) spectrum of **5a**



^{1}H NMR (400 MHz, CDCl3) spectrum of **6a**



^{13}C NMR (100 MHz, CDCl3) spectrum of **6a**

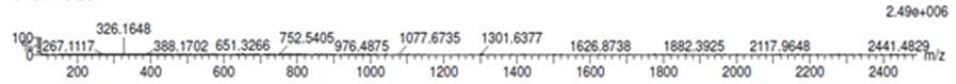


Compound 4a

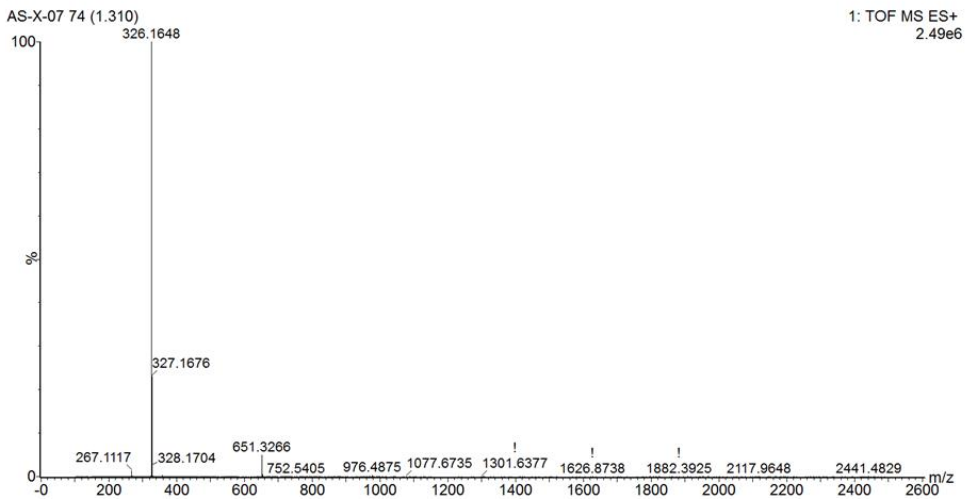
Elemental Composition Report

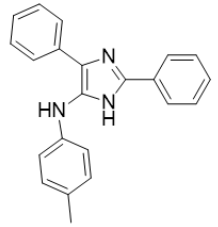
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10
AS-X-07 74 (1.310)
1: TOF MS ES+

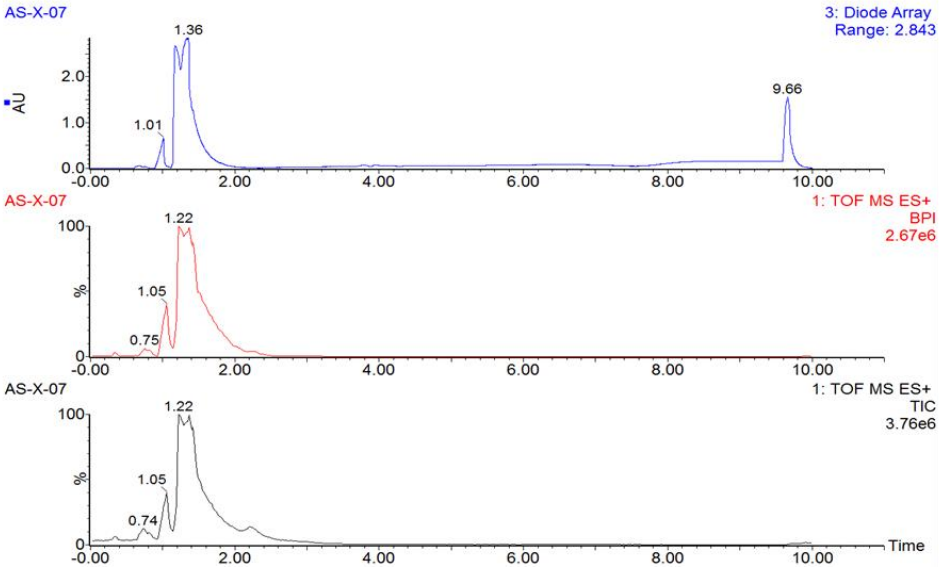


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
326.1648	326.1657	-0.9	-2.8	14.5	644.3	n/a	n/a	C22 H20 N3





$[M+H]^+$: $C_{22}H_{20}N_3$
Exact Mass: 326.1657

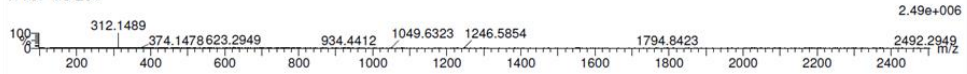


Compound 4b

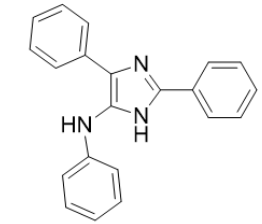
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

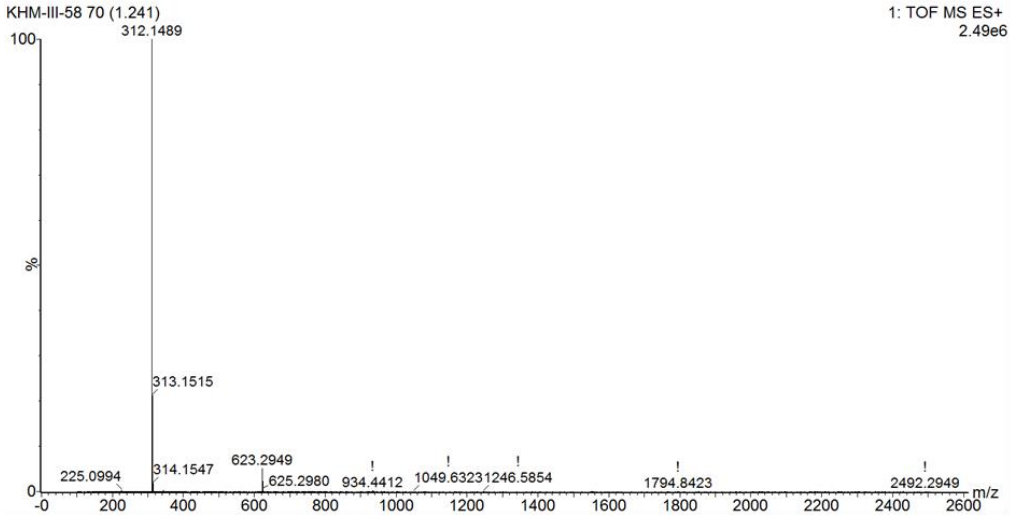
Monoisotopic Mass, Even Electron Ions
46 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10
KHM-III-58 70 (1.241)
1: TOF MS ES+

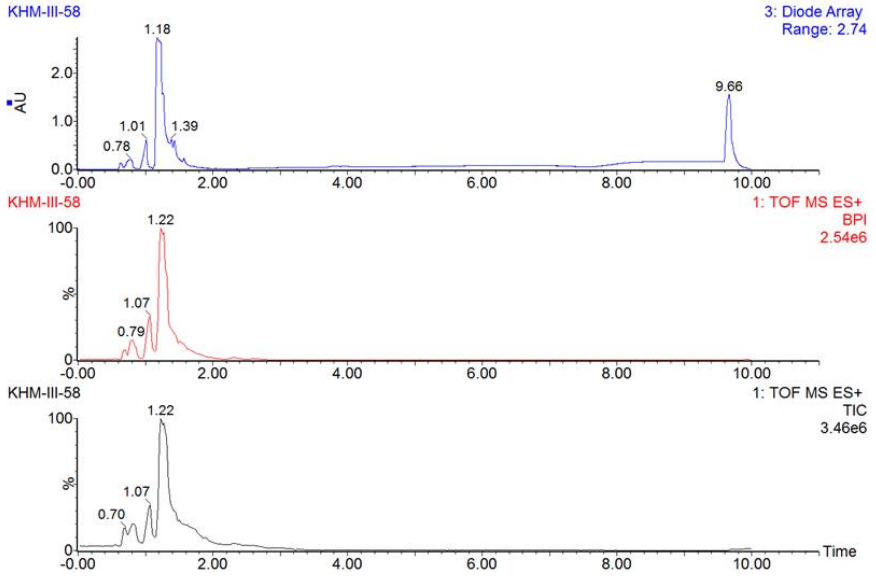


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
312.1489	312.1501	-1.2	-3.8	14.5	562.0	n/a	n/a	C21 H18 N3



$[M+H]^+$: $C_{21}H_{18}N_3$
Exact Mass: 312.1501



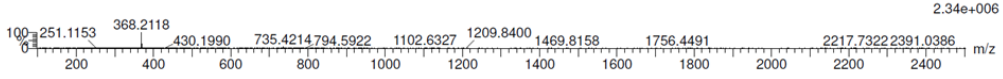


Compound 4c

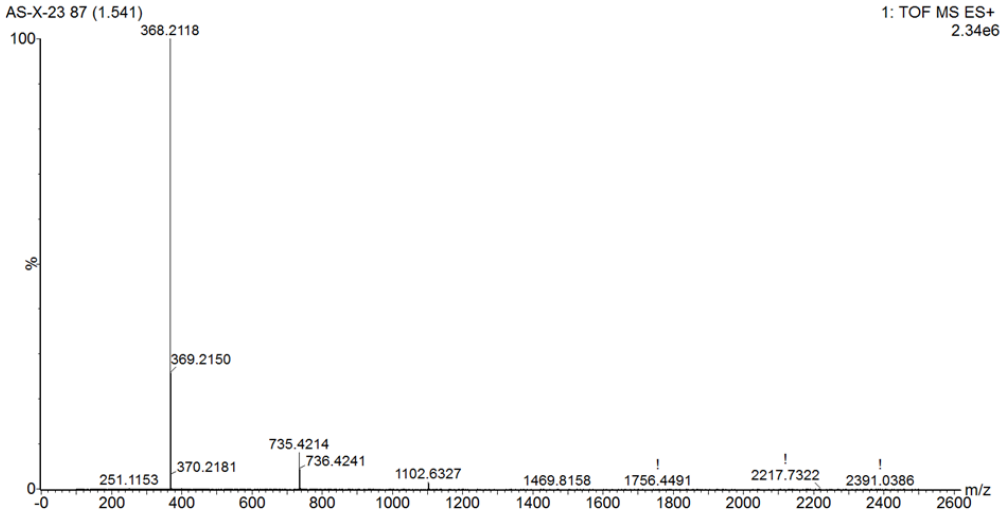
Elemental Composition Report

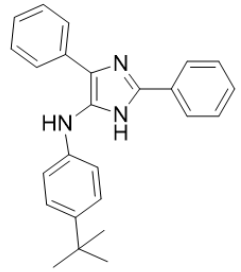
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
54 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10
AS-X-23 87 (1.541)
1: TOF MS ES+

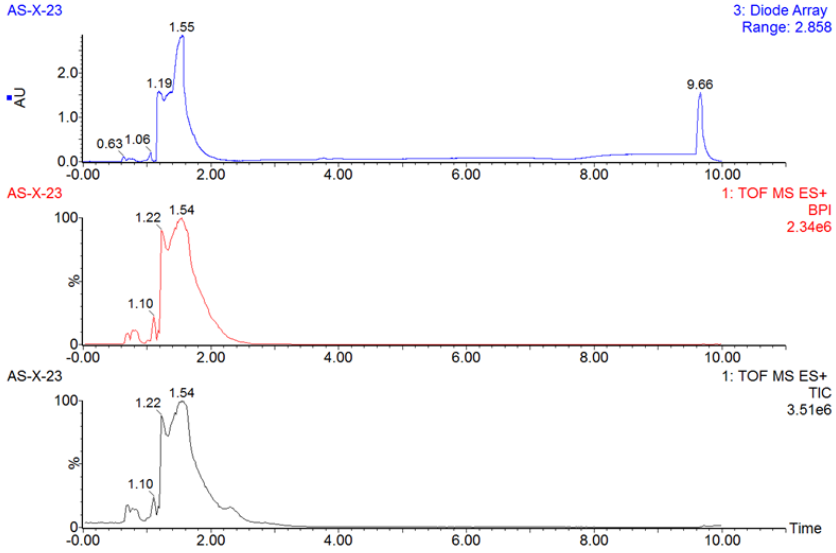


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
368.2118	368.2127	-0.9	-2.4	14.5	575.7	n/a	n/a	C25 H26 N3





$[M+H]^+$: $C_{25}H_{26}N_3$
Exact Mass: 368.2127

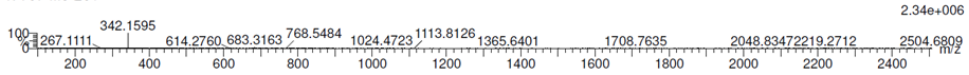


Compound 4d

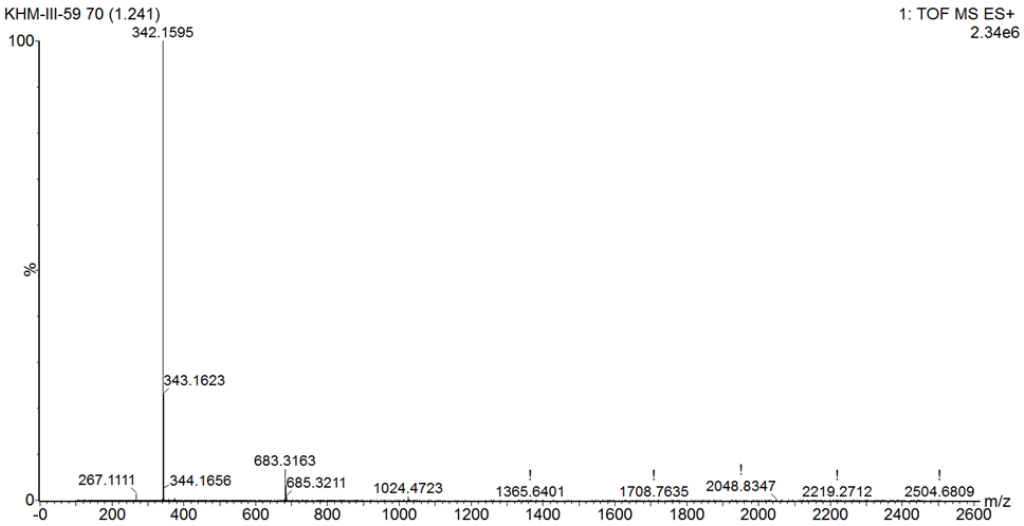
Elemental Composition Report

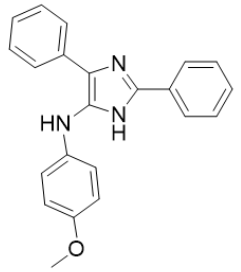
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
570 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20
KHM-III-59 70 (1.241)
1: TOF MS ES+

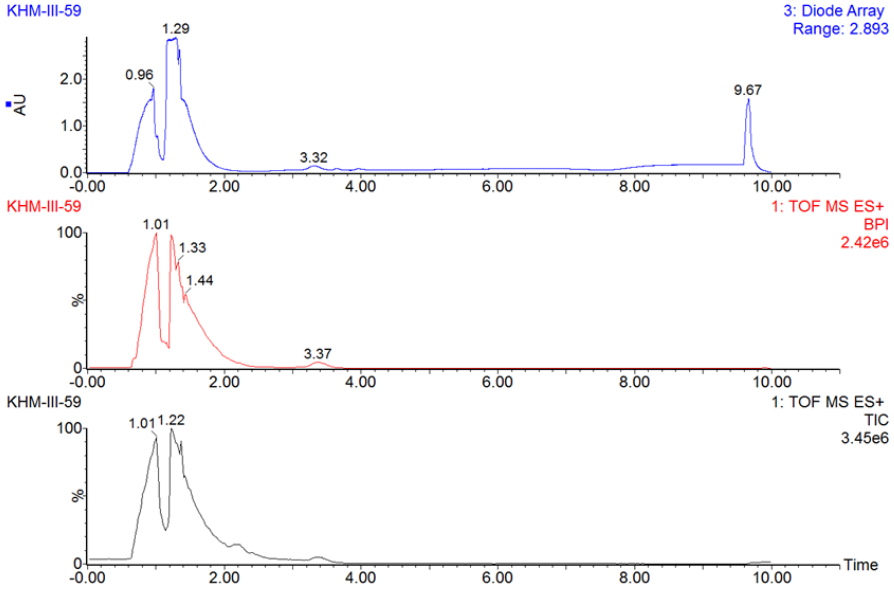


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
342.1595	342.1606	-1.1	-3.2	14.5	618.2	0.194	82.40	C22 H20 N3 O
	342.1566	2.9	8.5	10.5	619.8	1.761	17.19	C17 H20 N5 O3
	342.1553	4.2	12.3	5.5	623.7	5.605	0.37	C16 H24 N O7
	342.1638	-4.3	-12.6	6.5	626.4	8.363	0.02	C11 H20 N9 O4
	342.1625	-3.0	-8.8	1.5	626.8	8.784	0.02	C10 H24 N5 O8





$[M+H]^+$: $C_{22}H_{20}N_3O$
Exact Mass: 342.1606



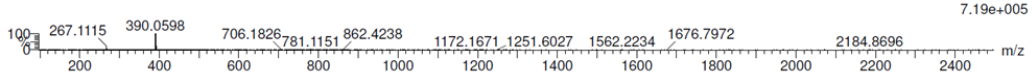
Compound 4e

Elemental Composition Report

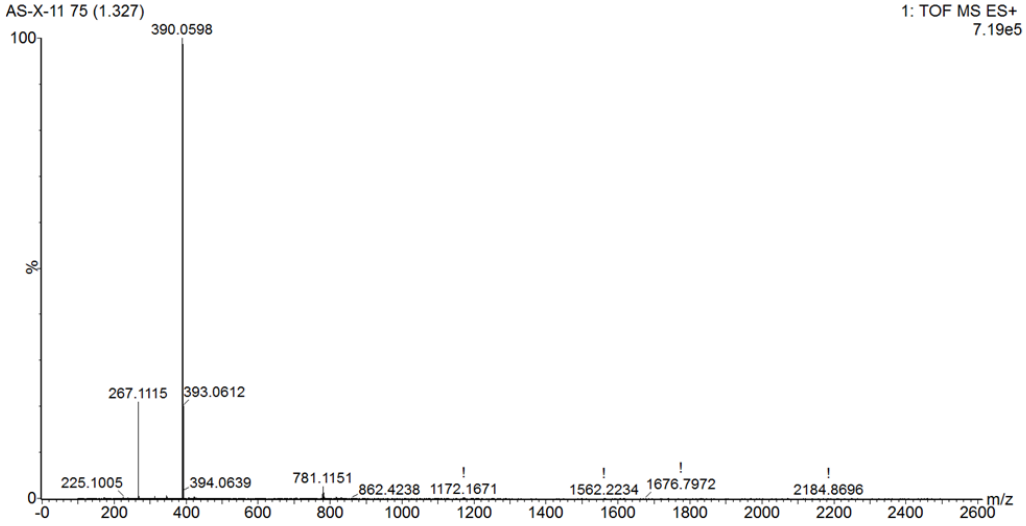
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

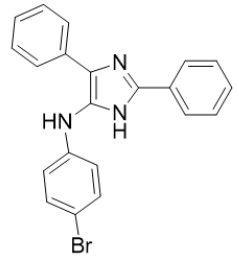
Monoisotopic Mass, Even Electron Ions
169 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

AS-X-11 75 (1.327)
1: TOF MS ES+

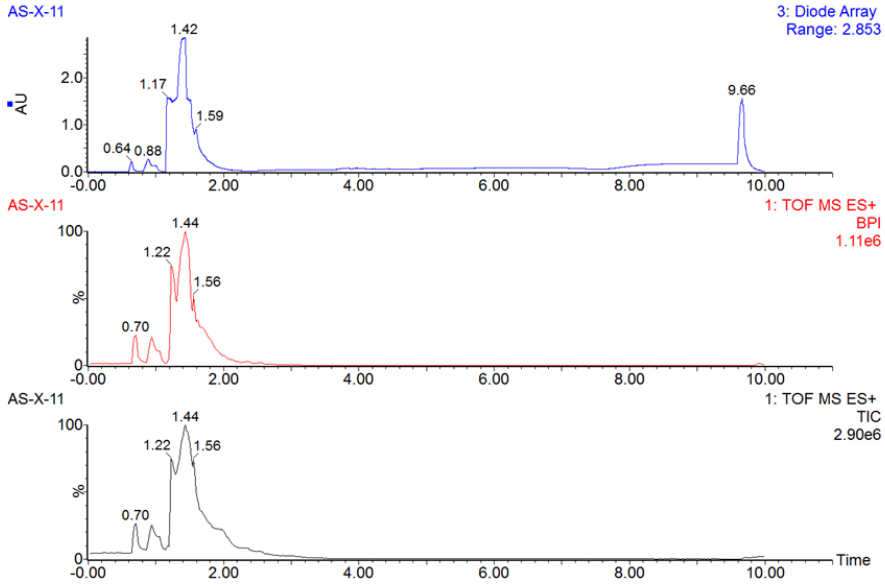


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
390.0598	390.0606	-0.8	-2.1	14.5	469.3	0.000	100.00	C21 H17 N3 Br
	390.0616	-1.8	-4.6	-0.5	480.1	10.814	0.00	C9 H26 N7 Br2





$[M+H]^+$: $C_{21}H_{17}N_3Br$
Exact Mass: 390.0606

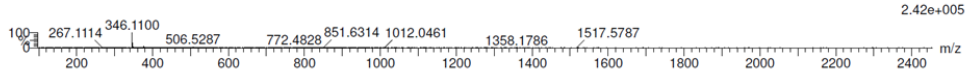


Compound 4f

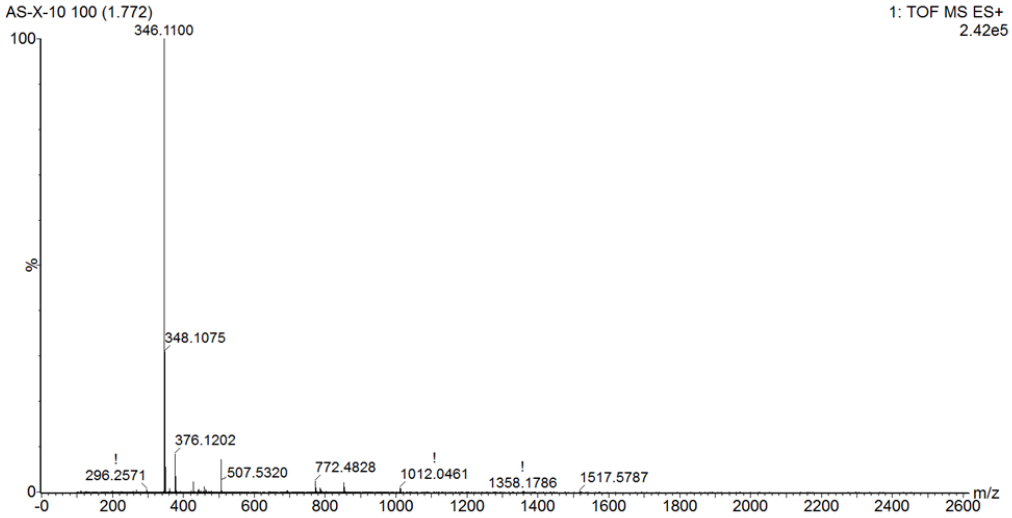
Elemental Composition Report

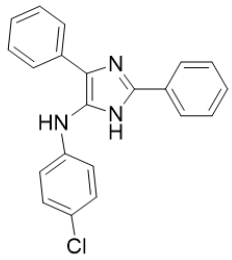
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
257 formula(e) evaluated with 5 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Cl: 0-8
AS-X-10 100 (1.772)
1: TOF MS ES+

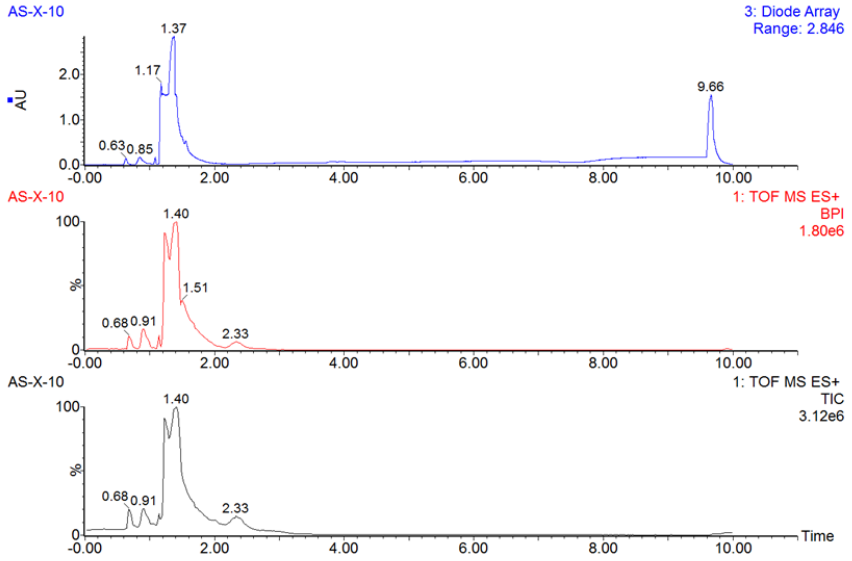


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
346.1100	346.1111	-1.1	-3.2	14.5	241.7	0.001	99.88	C21 H17 N3 Cl
	346.1129	-2.9	-8.4	9.5	248.5	6.800	0.11	C20 H22 N Cl2
	346.1062	3.8	11.0	6.5	252.2	10.559	0.00	C11 H18 N9 Cl2
	346.1081	1.9	5.5	1.5	252.9	11.207	0.00	C10 H23 N7 Cl3
	346.1093	0.7	2.0	19.5	259.2	17.523	0.00	C22 H12 N5





$[M+H]^+$: $C_{21}H_{17}N_3Cl$
Exact Mass: 346.1111

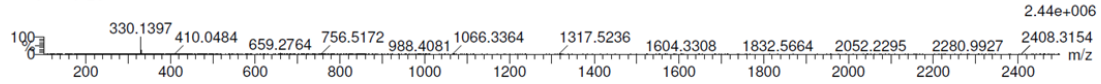


Compound 4g

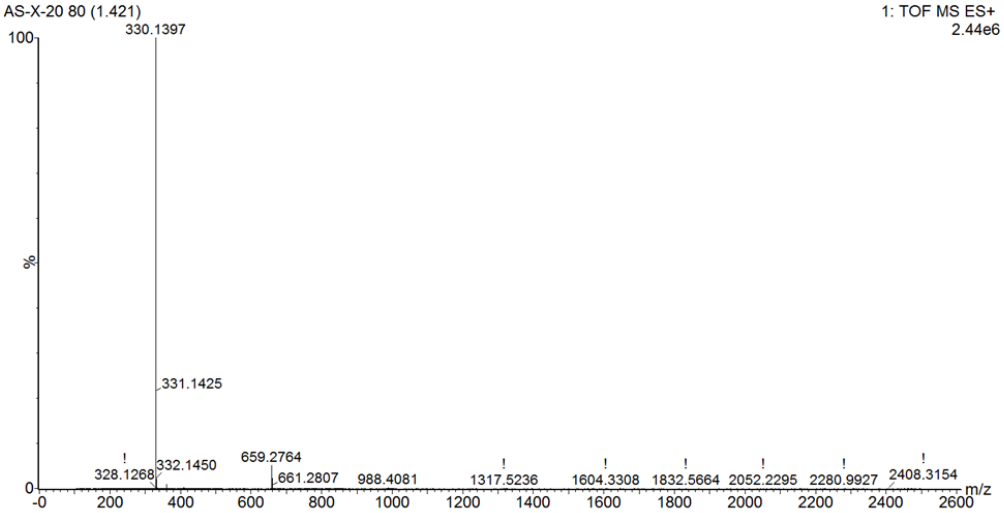
Elemental Composition Report

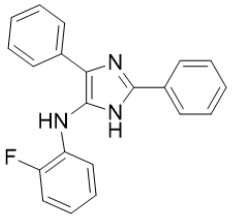
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
360 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10
AS-X-20 80 (1.421)
1: TOF MS ES+

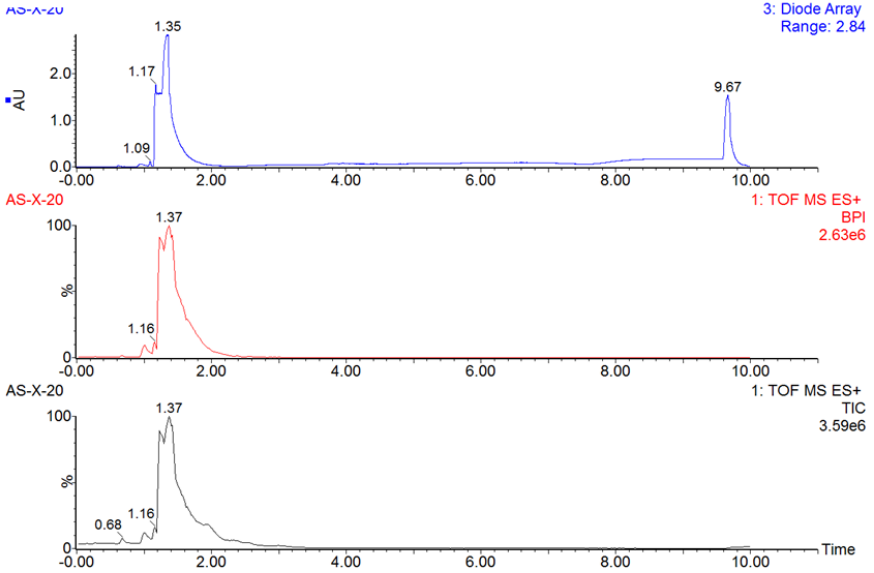


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
330.1397	330.1407	-1.0	-3.0	14.5	539.9	0.164	84.91	C21 H17 N3 F
	330.1405	-0.8	-2.4	3.5	541.7	1.967	13.99	C13 H18 N3 F6
	330.1403	-0.6	-1.8	7.5	544.3	4.513	1.10	C11 H15 N9 F3





$[M+H]^+$: $C_{21}H_{17}N_3F$
Exact Mass: 330.1407



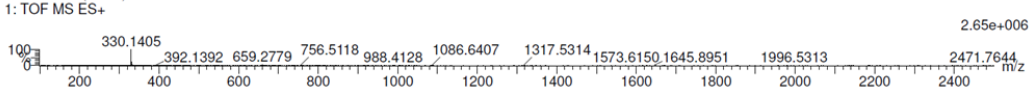
Compound 4h

Elemental Composition Report

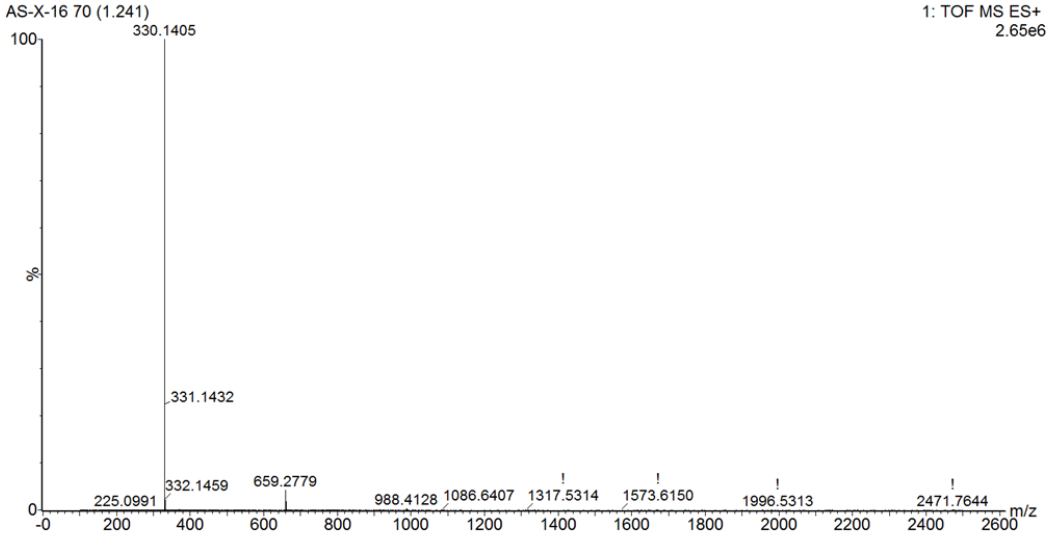
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

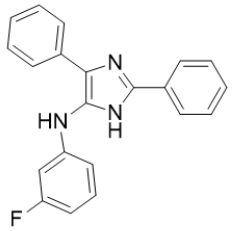
Monoisotopic Mass, Even Electron Ions
360 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10

AS-X-16 70 (1.241)
1: TOF MS ES+

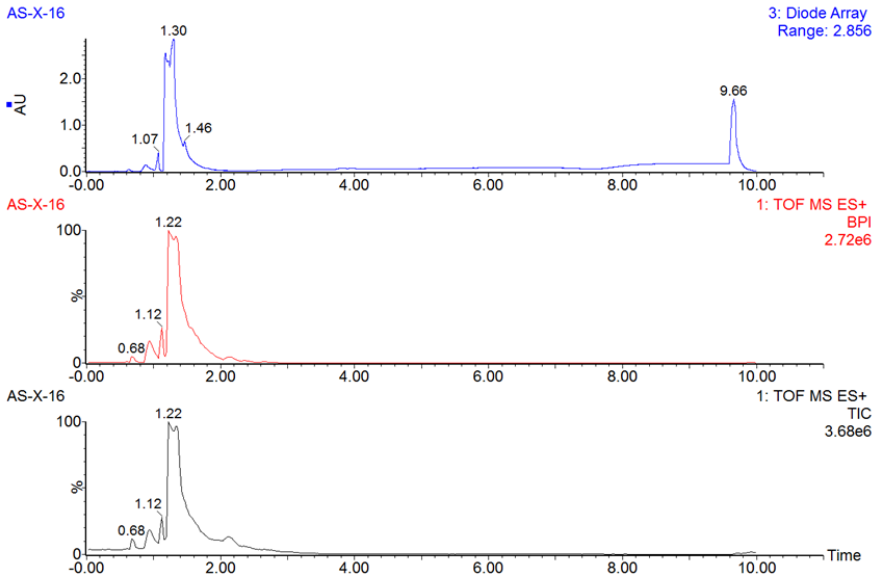


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
330.1405	330.1407	-0.2	-0.6	14.5	533.5	0.045	95.61	C21 H17 N3 F
	330.1405	0.0	0.0	3.5	536.6	3.155	4.26	C13 H18 N3 F6
	330.1403	0.2	0.6	7.5	540.1	6.659	0.13	C11 H15 N9 F3





$[M+H]^+$: $C_{21}H_{17}N_3F$
Exact Mass: 330.1407



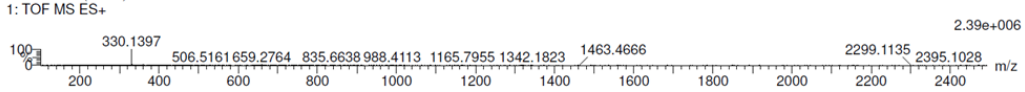
Compound 4i

Elemental Composition Report

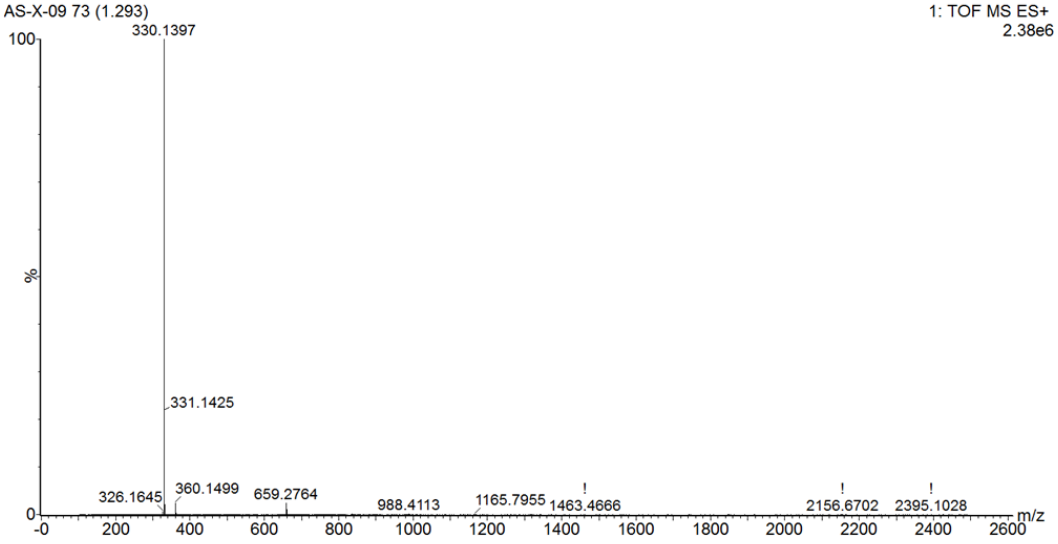
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

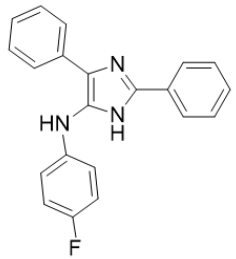
Monoisotopic Mass, Even Electron Ions
360 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10

AS-X-09 73 (1.293)
1: TOF MS ES+

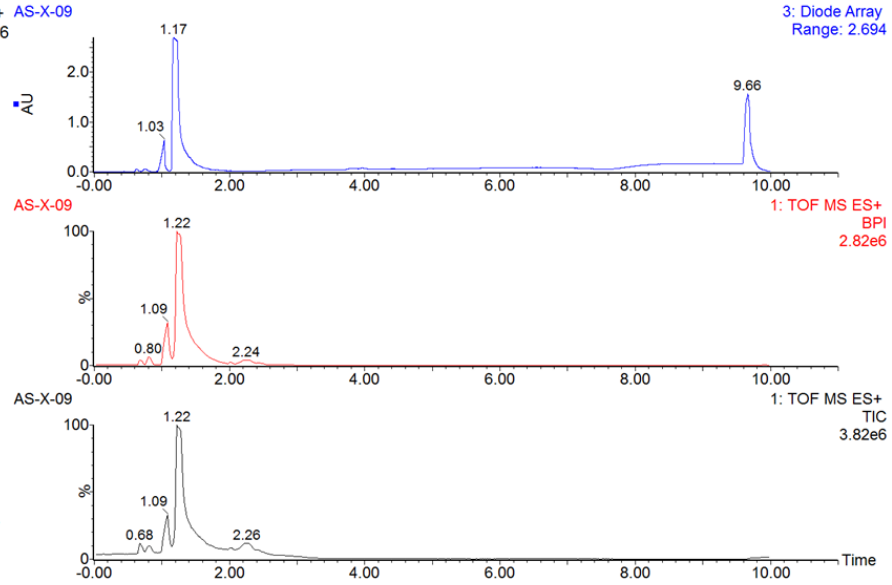


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
330.1397	330.1407	-1.0	-3.0	14.5	612.9	0.024	97.65	C21 H17 N3 F
	330.1405	-0.8	-2.4	3.5	616.6	3.762	2.32	C13 H18 N3 F6
	330.1403	-0.6	-1.8	7.5	621.3	8.470	0.02	C11 H15 N9 F3





$[M+H]^+$: $C_{21}H_{17}N_3F$
Exact Mass: 330.1407



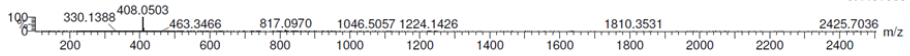
Compound 4j

Elemental Composition Report

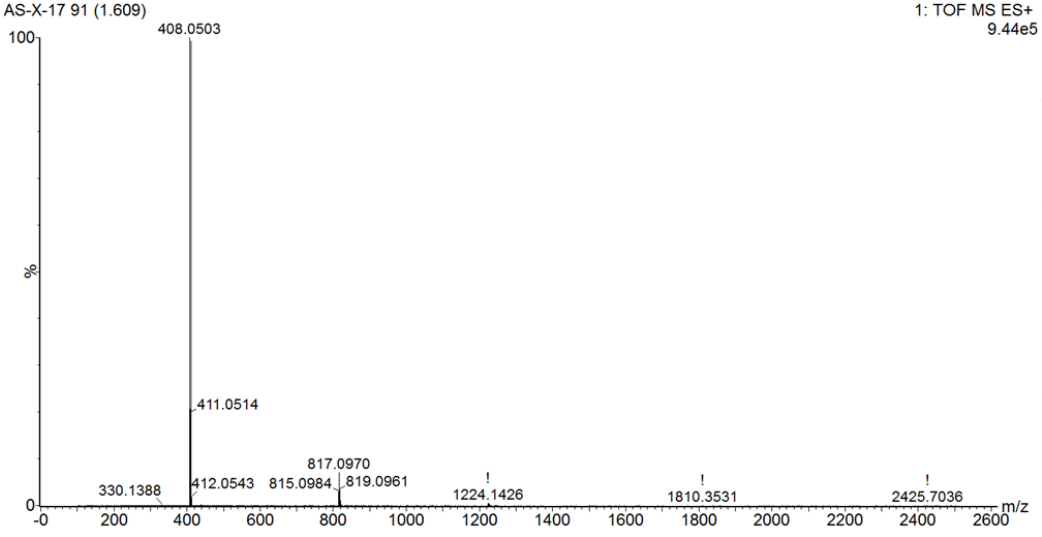
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

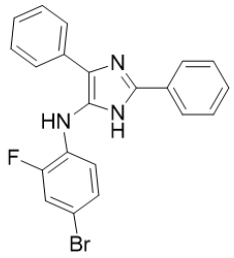
Monoisotopic Mass, Even Electron Ions
1178 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10 Br: 0-8

AS-X-17 91 (1.609)
1: TOF MS ES+
9.44e+005

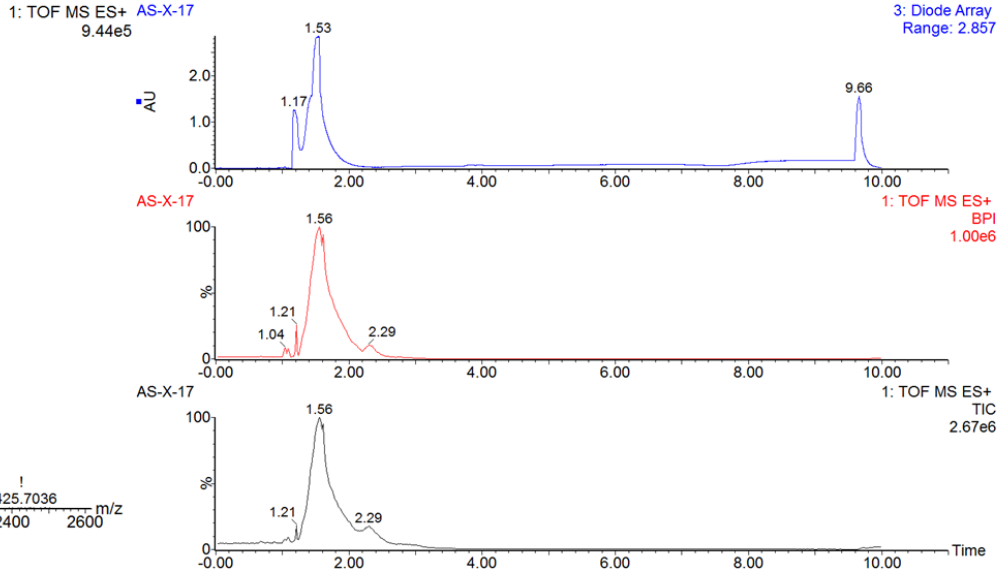


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.0503	408.0512	-0.9	-2.2	14.5	550.8	0.157	85.49	C21 H16 N3 F Br
	408.0510	-0.7	-1.7	3.5	552.6	2.025	13.20	C13 H17 N3 F6 Br
	408.0508	-0.5	-1.2	7.5	554.9	4.339	1.30	C11 H14 N9 F3 Br
	408.0522	-1.9	-4.7	-0.5	561.1	10.504	0.00	C9 H25 N7 F Br2
	408.0462	4.1	10.0	-0.5	561.5	10.888	0.00	C12 H26 N3 F2 Br2
	408.0495	0.8	2.0	11.5	571.9	21.313	0.00	C15 H6 N5 F8
	408.0497	0.6	1.5	22.5	572.0	21.427	0.00	C23 H5 N5 F3





$[M+H]^+$: $C_{21}H_{16}N_3FBr$
Exact Mass: 408.0512



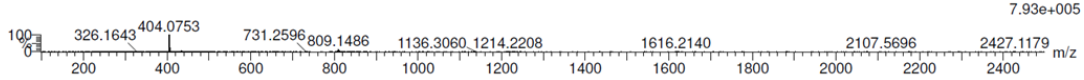
Compound 4k

Elemental Composition Report

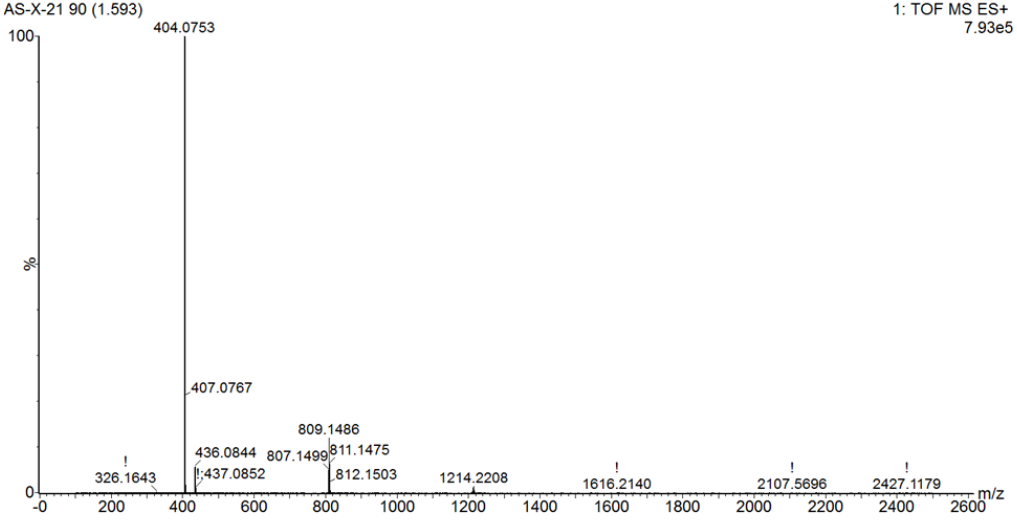
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
179 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

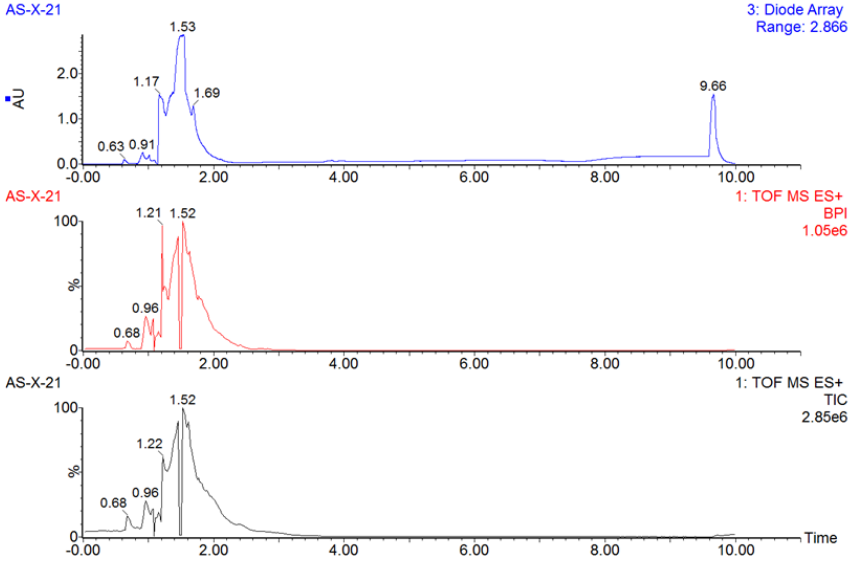
AS-X-21 90 (1.593)
1: TOF MS ES+
7.93e+005



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
404.0753	404.0762	-0.9	-2.2	14.5	558.4	0.000	100.00	C22 H19 N3 Br
	404.0773	-2.0	-4.9	-0.5	568.4	9.945	0.00	C10 H28 N7 Br2



$[M+H]^+$: $C_{22}H_{19}N_3Br$
Exact Mass: 404.0762



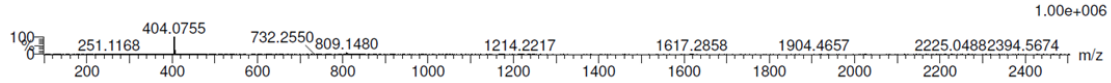
Compound 4l

Elemental Composition Report

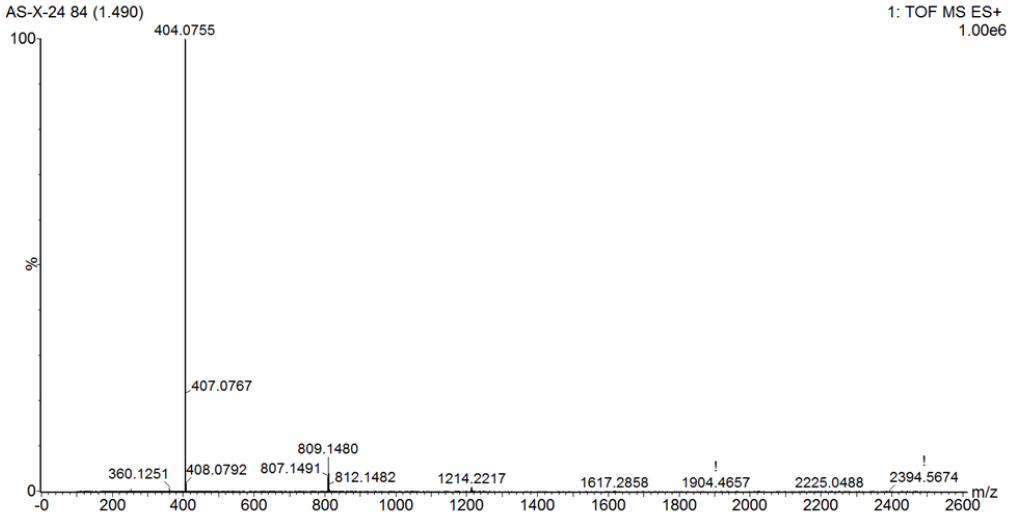
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

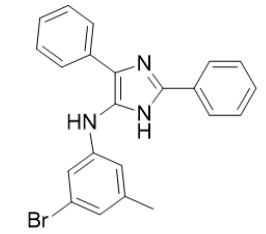
Monoisotopic Mass, Even Electron Ions
179 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

AS-X-24 84 (1.490)
1: TOF MS ES+

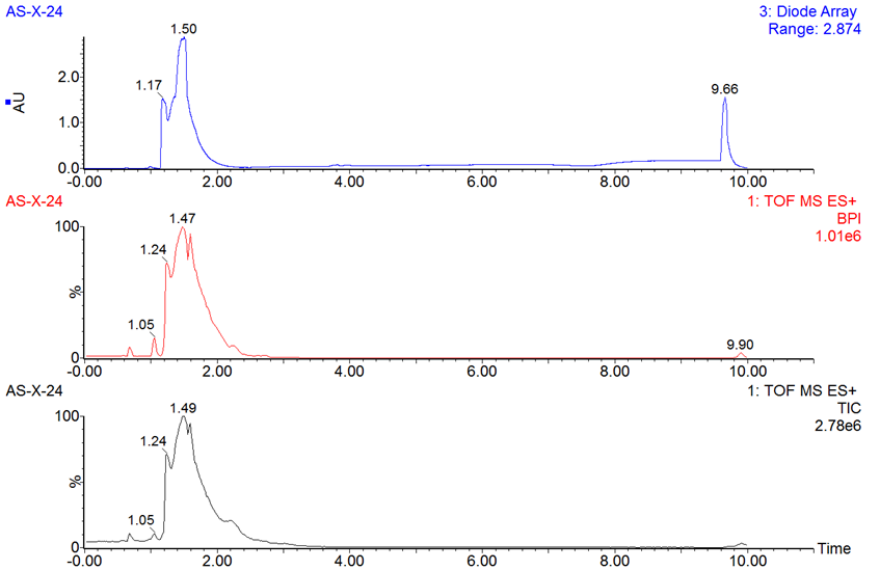


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
404.0755	404.0762	-0.7	-1.7	14.5	512.8	0.000	99.99	C22 H19 N3 Br
	404.0773	-1.8	-4.5	-0.5	522.6	9.843	0.01	C10 H28 N7 Br2





$[M+H]^+$: $C_{22}H_{19}N_3Br$
Exact Mass: 404.0762



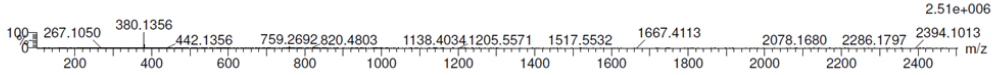
Compound 4m

Elemental Composition Report

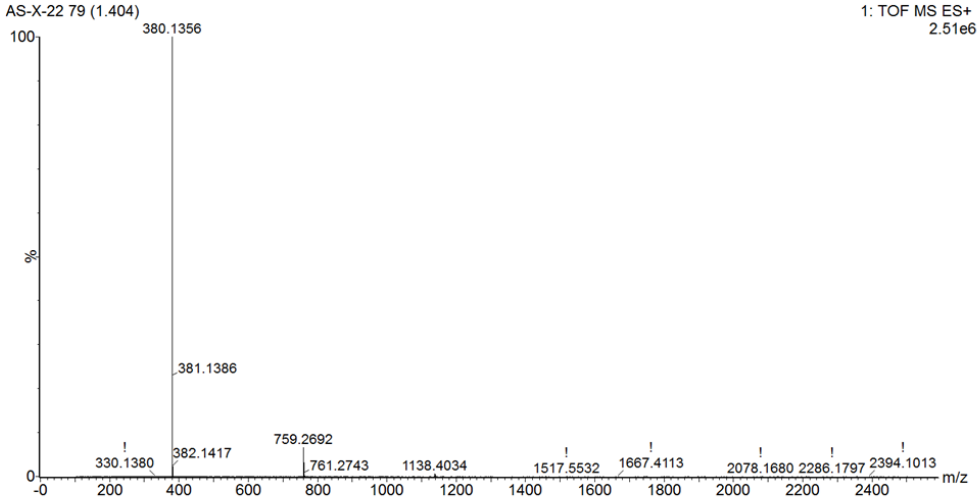
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

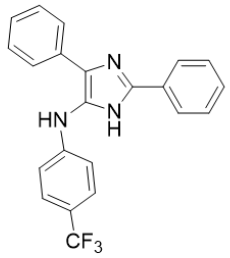
Monoisotopic Mass, Even Electron Ions
431 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10

AS-X-22 79 (1.404)
1: TOF MS ES+

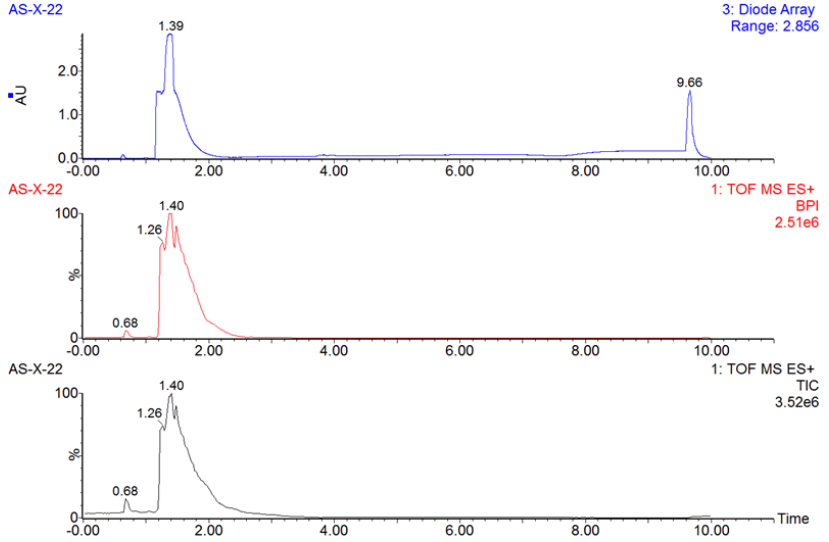


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
380.1356	380.1375	-1.9	-5.0	14.5	547.3	0.215	80.63	C22 H17 N3 F3
	380.1372	-1.6	-4.2	18.5	549.0	1.969	13.96	C20 H14 N9
	380.1373	-1.7	-4.5	3.5	550.4	3.314	3.64	C14 H18 N3 F8
	380.1311	4.5	11.8	18.5	551.7	4.572	1.03	C23 H15 N5 F
	380.1310	4.6	12.1	7.5	552.1	4.988	0.68	C15 H16 N5 F6
	380.1371	-1.5	-3.9	7.5	554.6	7.480	0.06	C12 H15 N9 F5





$[M+H]^+$: $C_{22}H_{17}N_3F_3$
Exact Mass:380.1375

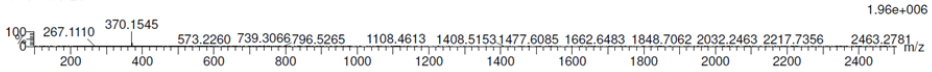


Compound 4n

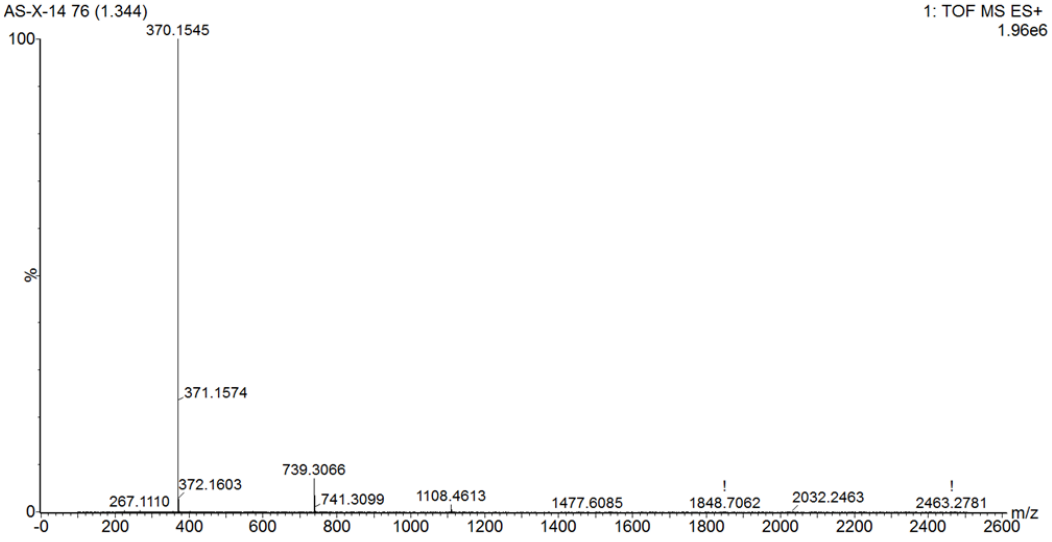
Elemental Composition Report

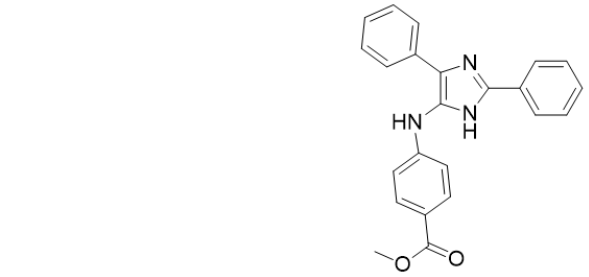
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
659 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20
AS-X-14 76 (1.344)
1: TOF MS ES+

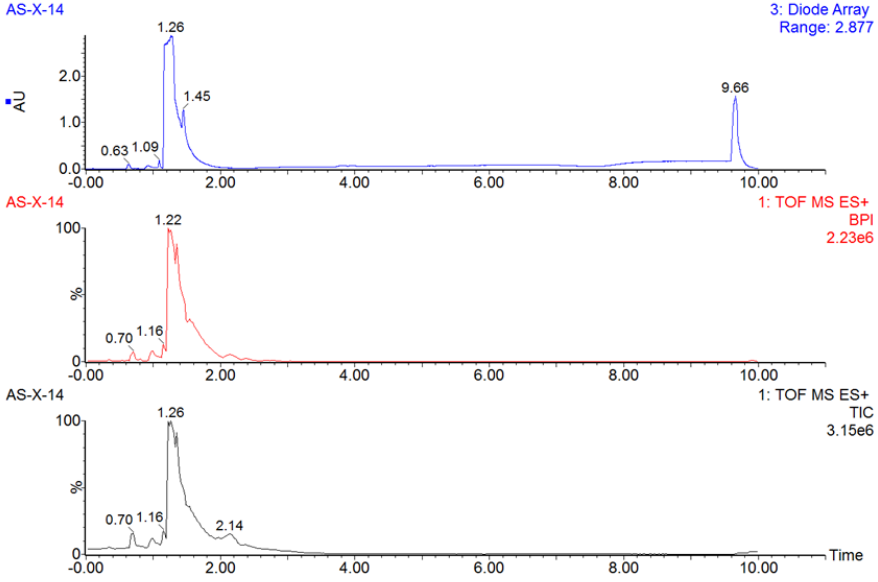


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
370.1545	370.1529	1.6	4.3	16.5	537.0	0.021	97.89	C19 H16 N9
	370.1515	3.0	8.1	11.5	541.2	4.195	1.51	C18 H20 N5 O4
	370.1556	-1.1	-3.0	15.5	542.1	5.139	0.59	C23 H20 N3 O2
	370.1502	4.3	11.6	6.5	545.8	8.811	0.01	C17 H24 N O8
	370.1587	-4.2	-11.3	7.5	548.5	11.494	0.00	C12 H20 N9 O5
	370.1574	-2.9	-7.8	2.5	548.8	11.794	0.00	C11 H24 N5 O9
	370.1534	1.1	3.0	-1.5	551.4	14.391	0.00	C6 H24 N7 O11





$[M+H]^+$: $C_{23}H_{20}N_3O_2$
Exact Mass: 370.1556

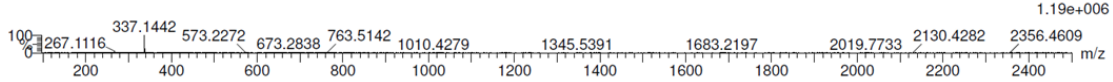


Compound 4o

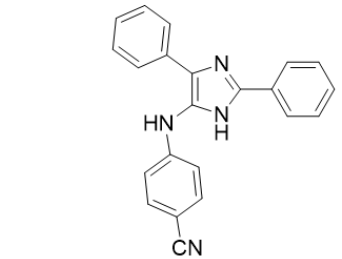
Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

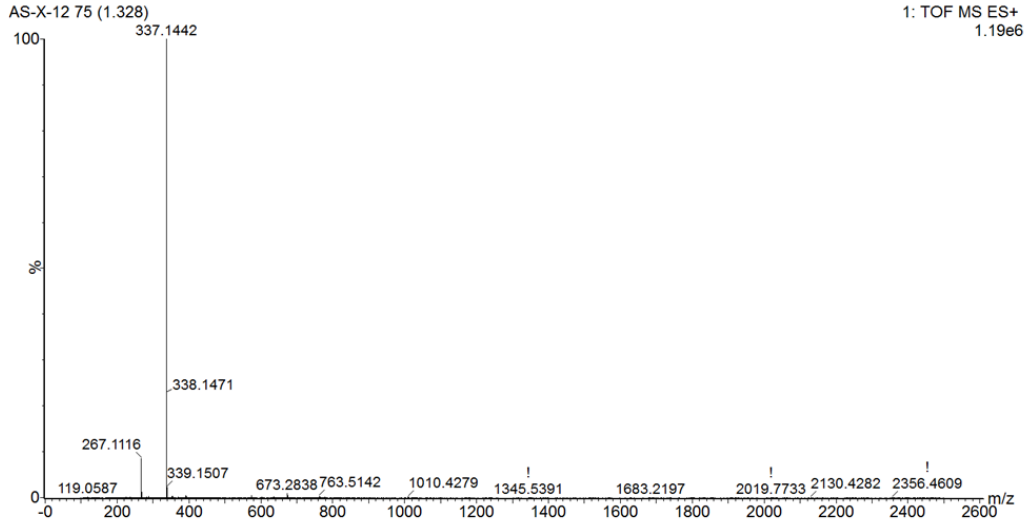
Monoisotopic Mass, Even Electron Ions
51 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10
AS-X-12 75 (1.328)
1: TOF MS ES+

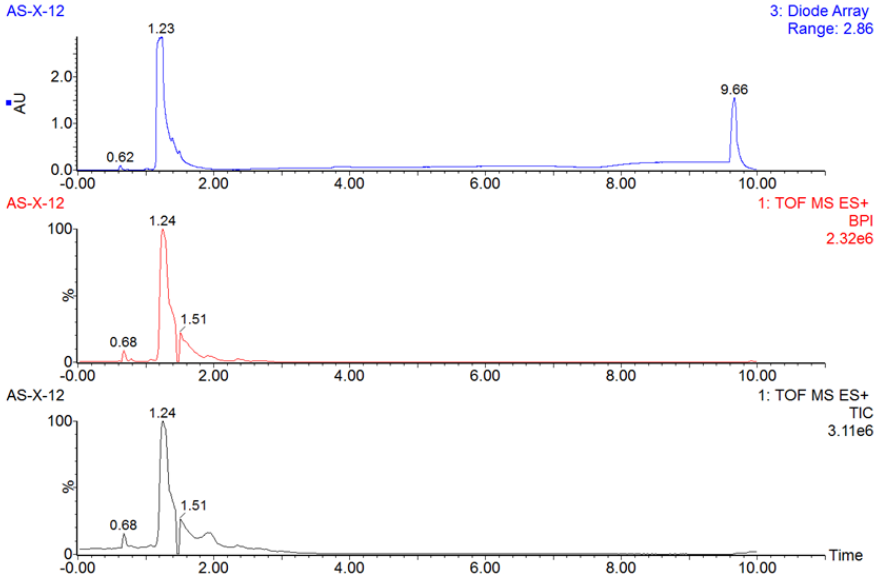


Minimum:		5.0	10.0	-1.5				
Maximum:				50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
337.1442	337.1453	-1.1	-3.3	16.5	433.1	n/a	n/a	C22 H17 N4



$[M+H]^+$: $C_{22}H_{17}N_4$
Exact Mass: 337.1453



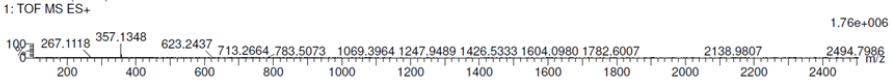


Compound 4p

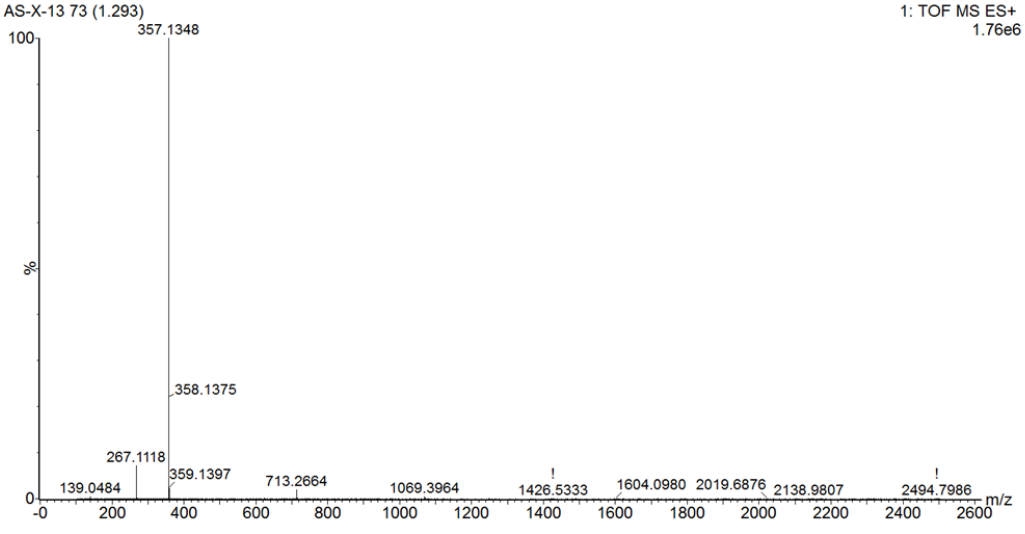
Elemental Composition Report

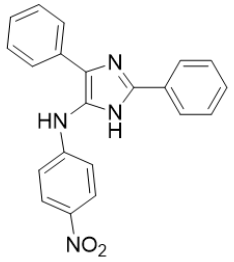
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
632 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20
AS-X-13 73 (1.293)
1: TOF MS ES+

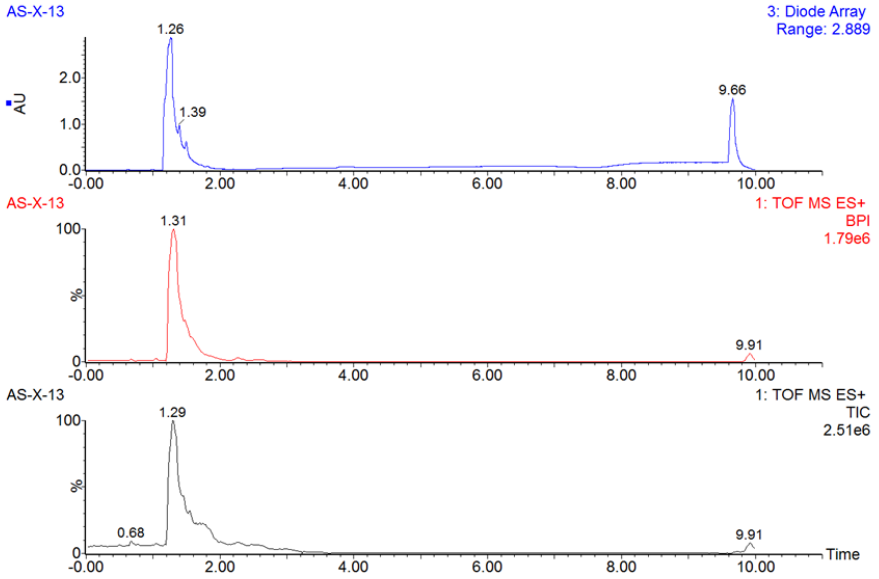


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
357.1348	357.1325	2.3	6.4	16.5	456.6	0.003	99.73	C17 H13 N10
	357.1311	3.7	10.4	11.5	462.8	6.202	0.20	C16 H17 N6 O4
	357.1352	-0.4	-1.1	15.5	464.3	7.708	0.04	C21 H17 N4 O2
	357.1338	1.0	2.8	10.5	465.1	8.547	0.02	C20 H21 O6
	357.1370	-2.2	-6.2	2.5	467.3	10.699	0.00	C9 H21 N6 O9
	357.1383	-3.5	-9.8	7.5	467.9	11.340	0.00	C10 H17 N10 O5
	357.1397	-4.9	-13.7	1.5	469.1	12.557	0.00	C13 H25 O11
	357.1392	-4.4	-12.3	19.5	470.2	13.646	0.00	C26 H17 N2
	357.1330	1.8	5.0	-1.5	471.8	15.254	0.00	C4 H21 N8 O11





$[M+H]^+$: $C_{21}H_{17}N_4O_2$
Exact Mass: 357.1352

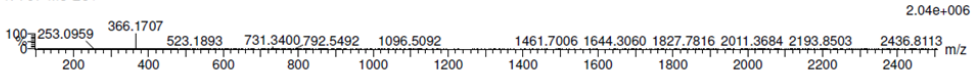


Compound 4q

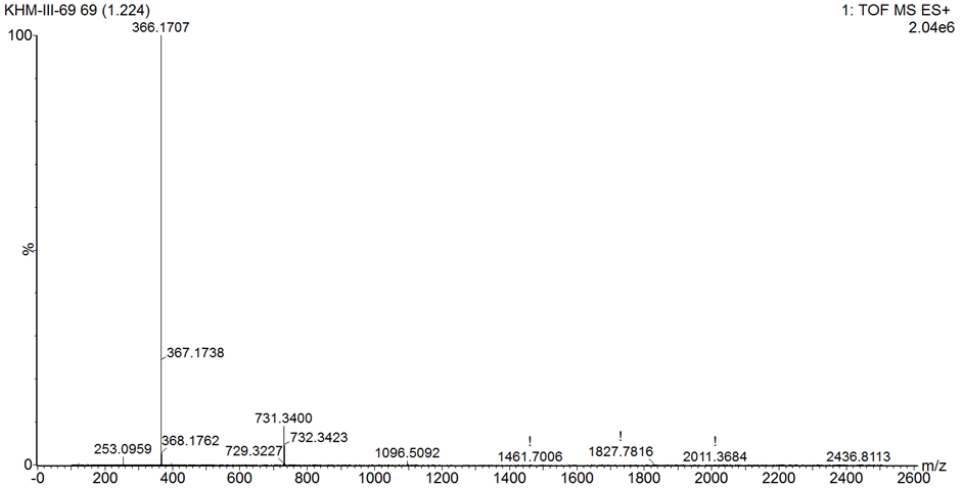
Elemental Composition Report Page 1

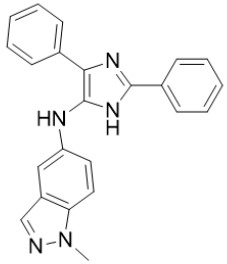
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
54 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10
KHM-III-69 69 (1.224)
1: TOF MS ES+

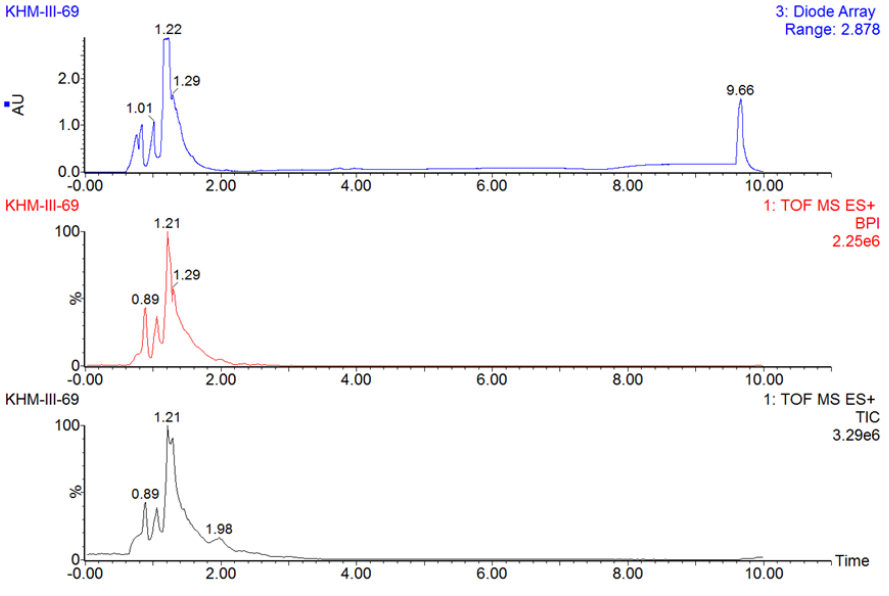


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
366.1707	366.1719	-1.2	-3.3	16.5	524.9	n/a	n/a	C23 H20 N5





$[M+H]^+$: $C_{23}H_{20}N_5$
Exact Mass: 366.1719



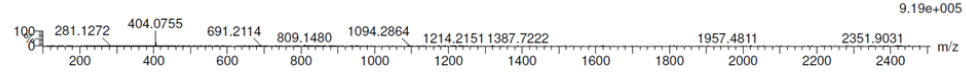
Compound 4r

Elemental Composition Report

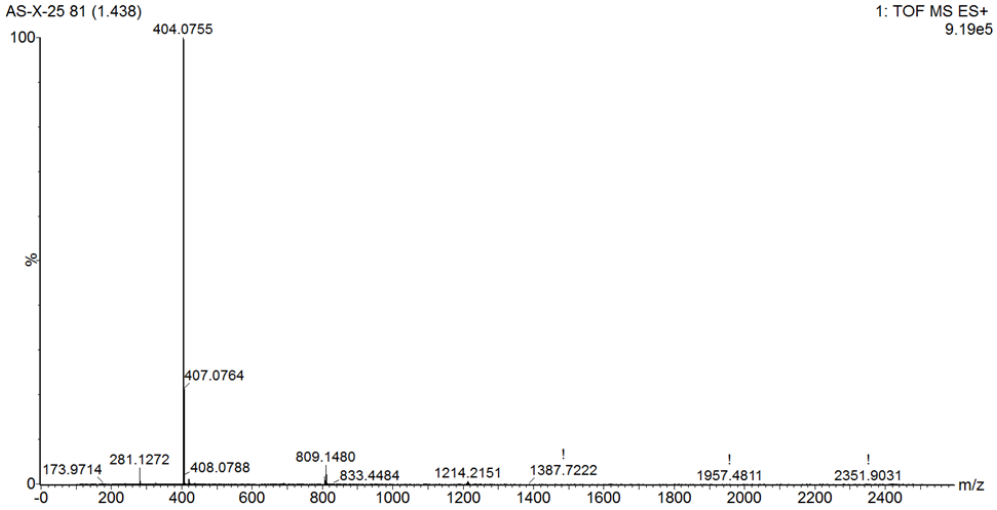
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

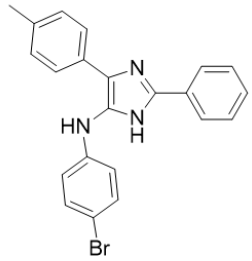
Monoisotopic Mass, Even Electron Ions
179 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

AS-X-25 81 (1.438)
1: TOF MS ES+
9.19e+005

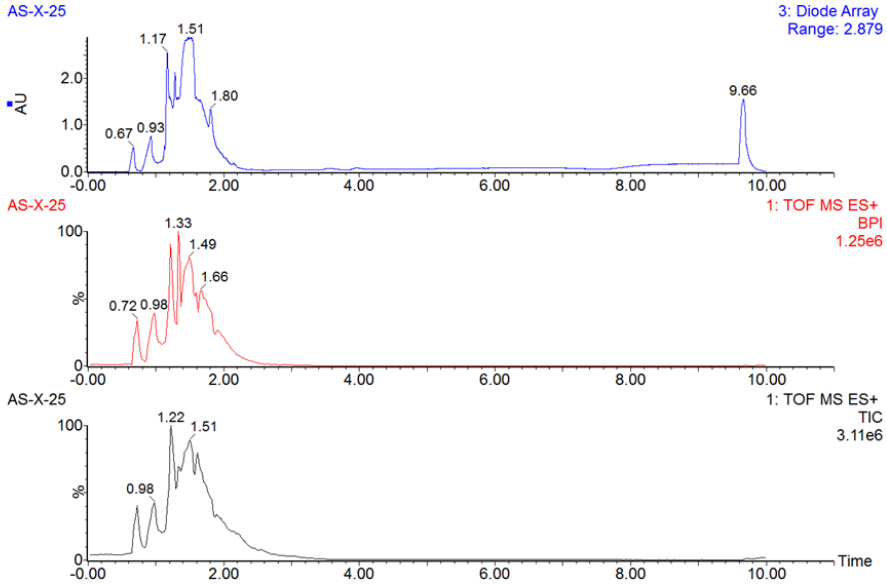


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
404.0755	404.0762	-0.7	-1.7	14.5	523.4	0.000	100.00	C22 H19 N3 Br
	404.0773	-1.8	-4.5	-0.5	534.2	10.763	0.00	C10 H28 N7 Br2





$[M+H]^+$: $C_{22}H_{19}BrN_3$
Exact Mass: 404.0762



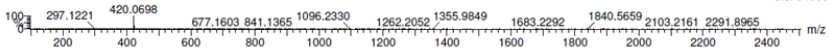
Compound 4s

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

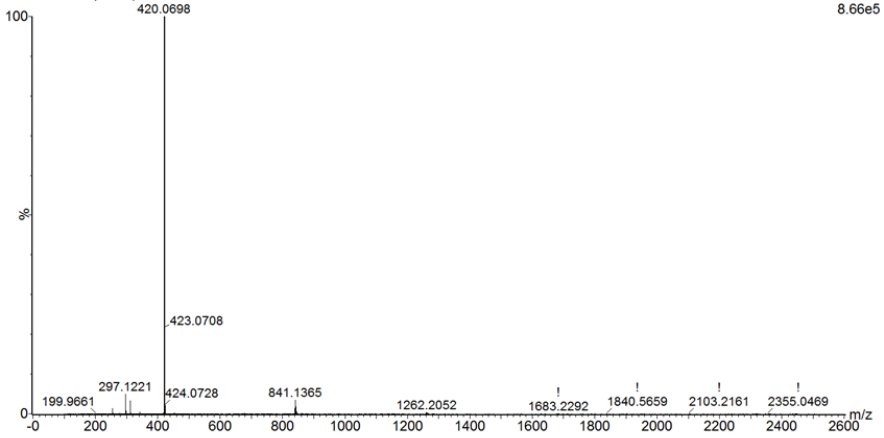
Monoisotopic Mass, Even Electron Ions
1896 formula(e) evaluated with 17 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

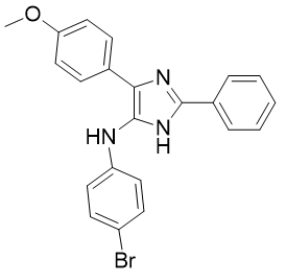
KHM-III-70 74 (1.310)
1: TOF MS ES+
8.67e+005



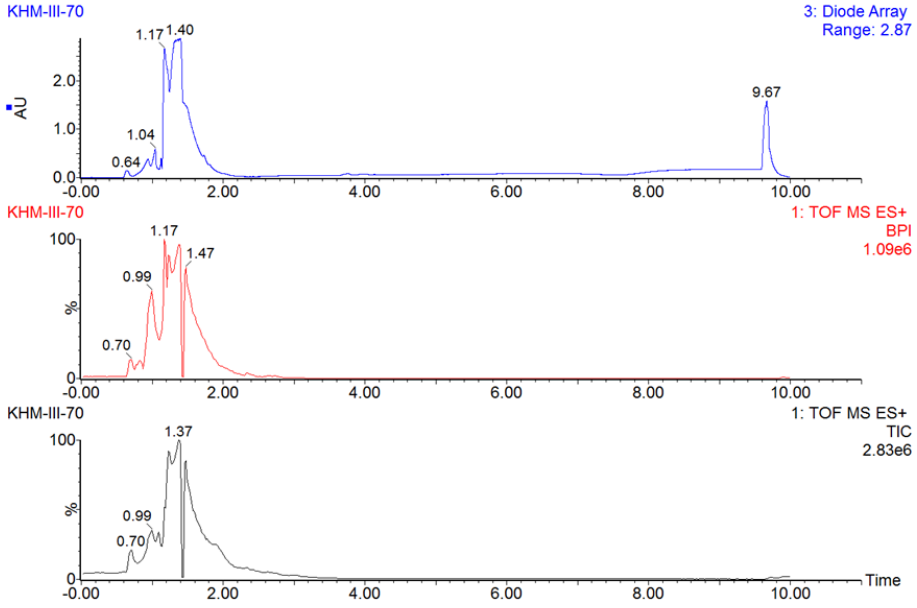
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
420.0698	420.0671	2.7	6.4	10.5	588.3	0.017	98.28	C17 H19 N5 O3 Br
	420.0712	-1.4	-3.3	14.5	592.5	4.190	1.51	C22 H19 N3 O Br
	420.0658	4.0	9.5	5.5	594.6	6.320	0.18	C16 H23 N O7 Br
	420.0730	-3.2	-7.6	1.5	597.3	9.017	0.01	C10 H23 N5 O8 Br
	420.0743	-4.5	-10.7	6.5	597.6	9.222	0.01	C11 H19 N9 O4 Br
	420.0722	-2.4	-5.7	-0.5	601.4	13.042	0.00	C10 H28 N7 O Br2
	420.0650	4.8	11.4	3.5	603.0	14.693	0.00	C16 H28 N3 Br2
	420.0652	4.6	11.0	13.5	612.4	24.043	0.00	C13 H10 N9 O8
	420.0738	-4.0	-9.5	3.5	612.4	24.081	0.00	C10 H18 N3 O15
	420.0698	0.0	0.0	-0.5	612.5	24.175	0.00	C5 H18 N5 O17
	420.0679	1.9	4.5	12.5	612.5	24.199	0.00	C17 H14 N3 O10
	420.0693	0.5	1.2	17.5	612.6	24.221	0.00	C18 H10 N7 O6
	420.0711	-1.3	-3.1	4.5	612.6	24.235	0.00	C6 H14 N9 O13
	420.0719	-2.1	-5.0	16.5	612.8	24.509	0.00	C22 H14 N O8
	420.0733	-3.5	-8.3	21.5	612.9	24.558	0.00	C23 H10 N5 O4
	420.0746	-4.8	-11.4	26.5	612.9	24.569	0.00	C24 H6 N9
	420.0661	3.7	8.8	25.5	613.1	24.816	0.00	C29 H10 N O3

KHM-III-70 74 (1.310)
1: TOF MS ES+
8.66e5





$[M+H]^+$: $C_{22}H_{19}N_3OBr$
Exact Mass: 420.0712



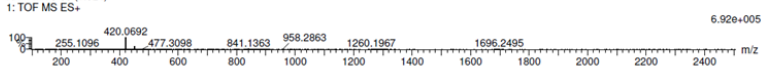
Compound 4t

Elemental Composition Report

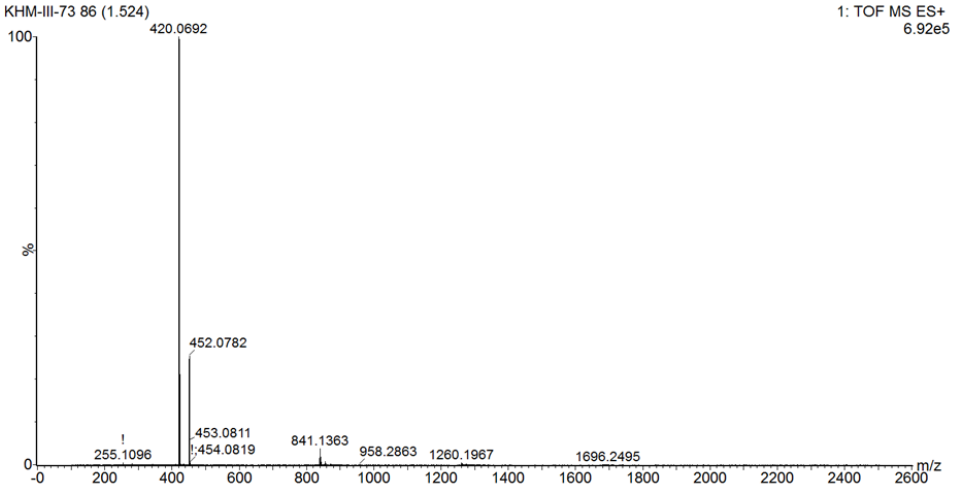
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

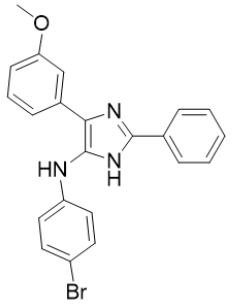
Monoisotopic Mass, Even Electron Ions
1896 formula(e) evaluated with 15 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

KHM-III-73 86 (1.524)
1: TOF MS ES+

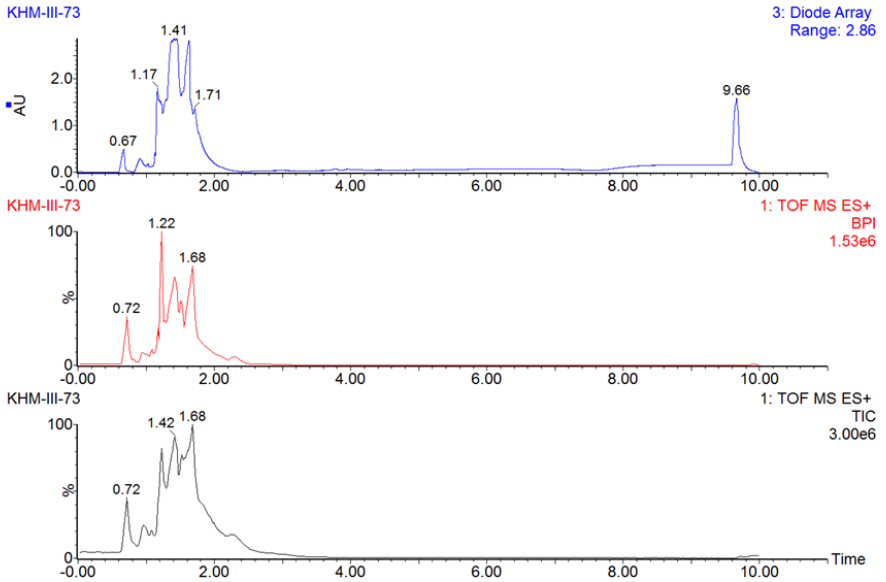


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
420.0692	420.0671	2.1	5.0	10.5	482.1	0.063	93.92	C17 H19 N5 O3 Br
	420.0712	-2.0	-4.8	14.5	484.9	2.904	5.48	C22 H19 N3 O Br
	420.0658	3.4	8.1	5.5	487.2	5.134	0.59	C16 H23 N O7 Br
	420.0730	-3.8	-9.0	1.5	491.0	8.937	0.01	C10 H23 N5 O8 Br
	420.0722	-3.0	-7.1	-0.5	495.1	13.059	0.00	C10 H28 N7 O Br2
	420.0650	4.2	10.0	3.5	495.4	13.373	0.00	C16 H28 N3 Br2
	420.0652	4.0	9.5	13.5	505.2	23.148	0.00	C13 H10 N9 O8
	420.0738	-4.6	-11.0	3.5	505.2	23.202	0.00	C10 H18 N3 O15
	420.0679	1.3	3.1	12.5	505.3	23.295	0.00	C17 H14 N3 O10
	420.0698	-0.6	-1.4	-0.5	505.3	23.301	0.00	C5 H18 N5 O17
	420.0693	-0.1	-0.2	17.5	505.4	23.325	0.00	C18 H10 N7 O6
	420.0711	-1.9	-4.5	4.5	505.4	23.373	0.00	C6 H14 N9 O13
	420.0719	-2.7	-6.4	16.5	505.6	23.605	0.00	C22 H14 N O8
	420.0733	-4.1	-9.8	21.5	505.7	23.661	0.00	C23 H10 N5 O4
	420.0661	3.1	7.4	25.5	505.9	23.895	0.00	C29 H10 N O3





$[M+H]^+$: $C_{22}H_{19}N_3OBr$
Exact Mass: 420.0712



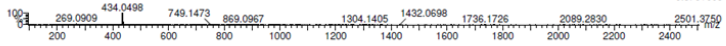
Compound 4u

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

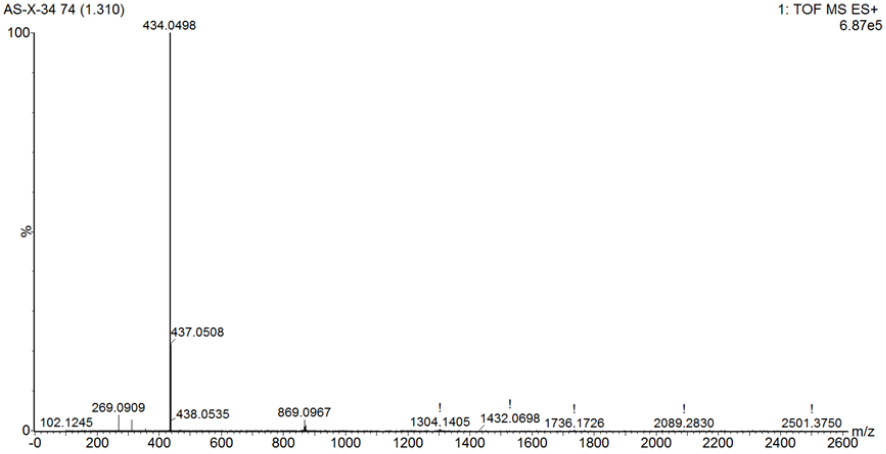
Monoisotopic Mass, Even Electron Ions
2060 formula(e) evaluated with 21 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

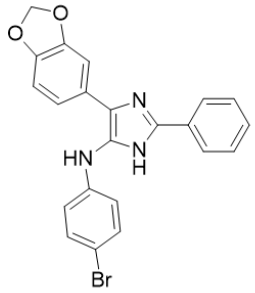
AS-X-34 74 (1.310)
1: TOF MS ES+
6.87e+005



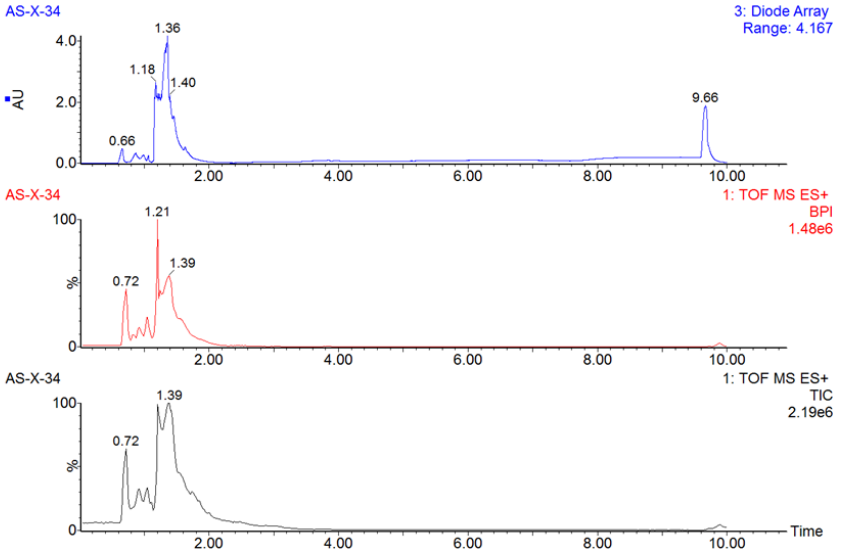
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
434.0498	434.0477	2.1	4.8	16.5	446.5	0.071	93.12	C18 H13 N9 Br
	434.0464	3.4	7.8	11.5	449.4	3.026	4.85	C17 H17 N5 O4 Br
	434.0504	-0.6	-1.4	15.5	450.3	3.919	1.99	C22 H17 N3 O2 Br
	434.0451	4.7	10.8	6.5	454.6	8.140	0.03	C16 H21 N O8 Br
	434.0523	-2.5	-5.8	2.5	455.8	9.374	0.01	C10 H21 N5 O9 Br
	434.0536	-3.8	-8.8	7.5	456.2	9.761	0.01	C11 H17 N9 O5 Br
	434.0544	-4.6	-10.6	19.5	457.0	10.600	0.00	C27 H17 N Br
	434.0482	1.6	3.7	-1.5	459.6	13.223	0.00	C5 H21 N7 O11 Br
	434.0515	-1.7	-3.9	0.5	460.0	13.564	0.00	C10 H26 N7 O2 Br2
	434.0542	-4.4	-10.1	-0.5	462.0	15.548	0.00	C14 H30 N O4 Br2
	434.0531	-3.3	-7.6	4.5	471.1	24.636	0.00	C10 H16 N3 O16
	434.0544	-4.6	-10.6	9.5	471.2	24.740	0.00	C11 H12 N7 O12
	434.0490	0.8	1.8	0.5	471.2	24.745	0.00	C5 H16 N5 O18
	434.0472	2.6	6.0	13.5	471.2	24.754	0.00	C17 H12 N3 O11
	434.0485	1.3	3.0	18.5	471.2	24.763	0.00	C18 H8 N7 O7
	434.0504	-0.6	-1.4	5.5	471.3	24.835	0.00	C6 H12 N9 O14
	434.0512	-1.4	-3.2	17.5	471.5	25.040	0.00	C22 H12 N O9
	434.0525	-2.7	-6.2	22.5	471.5	25.095	0.00	C23 H8 N5 O5
	434.0539	-4.1	-9.4	27.5	471.5	25.103	0.00	C24 H4 N9 O
	434.0467	3.1	7.1	31.5	471.8	25.359	0.00	C30 H4 N5
	434.0453	4.5	10.4	26.5	471.8	25.366	0.00	C29 H8 N O4

AS-X-34 74 (1.310)
1: TOF MS ES+
6.87e5





$[M+H]^+$: $C_{22}H_{17}N_3O_2Br$
Exact Mass: 434.0504



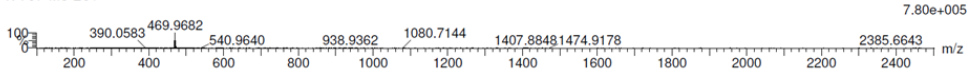
Compound 4v

Elemental Composition Report

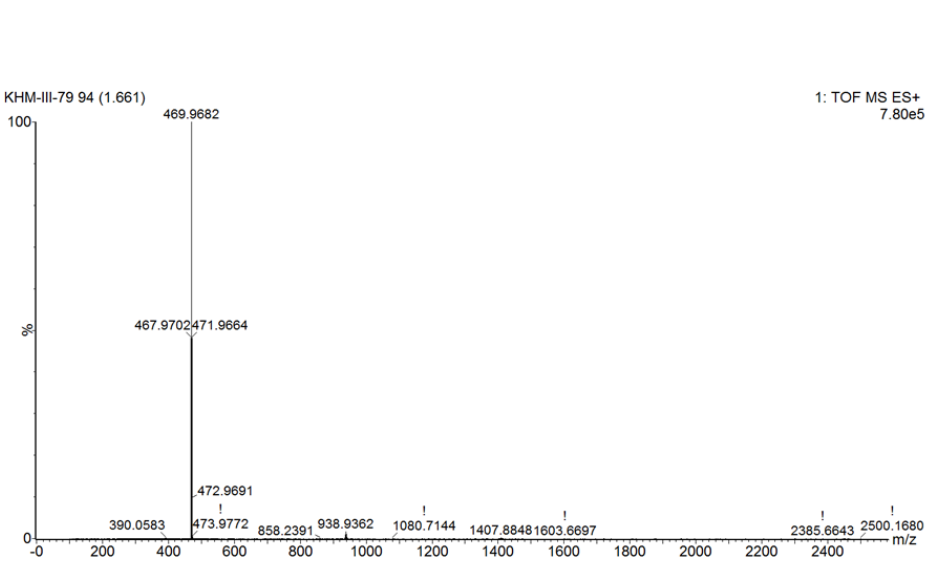
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
232 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

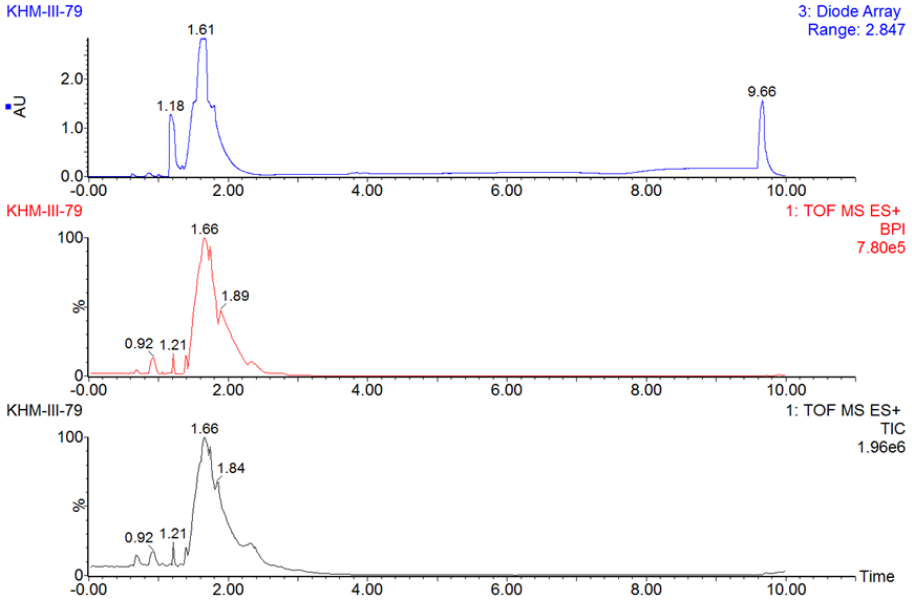
KHM-III-79 94 (1.661)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
467.9702	467.9711	-0.9	-1.9	14.5	403.8	0.002	99.82	C21 H16 N3 Br2
	467.9722	-2.0	-4.3	-0.5	410.2	6.347	0.18	C9 H25 N7 Br3



$[M+H]^+$: $C_{21}H_{16}N_3Br_2$
Exact Mass: 467.9711



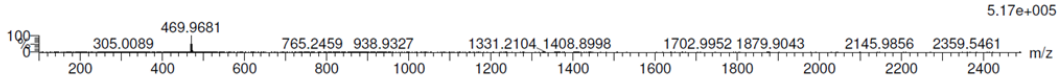
Compound 4w

Elemental Composition Report

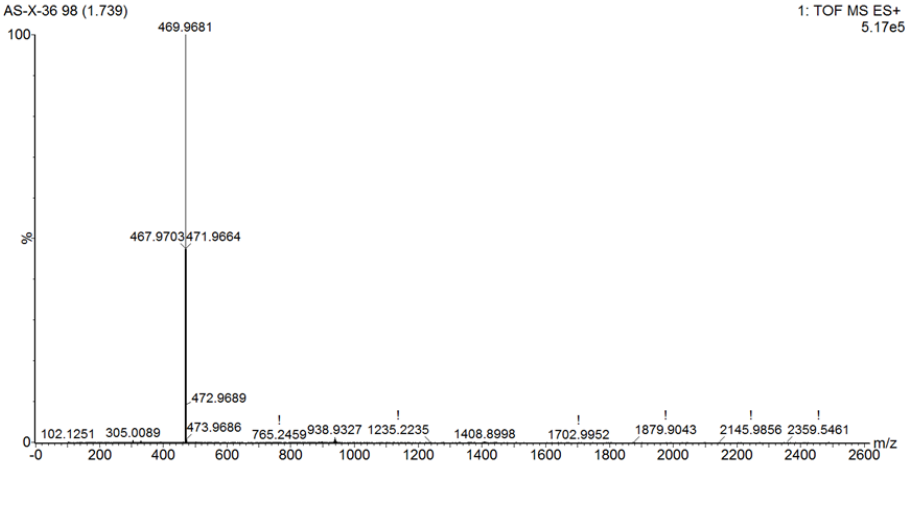
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
232 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

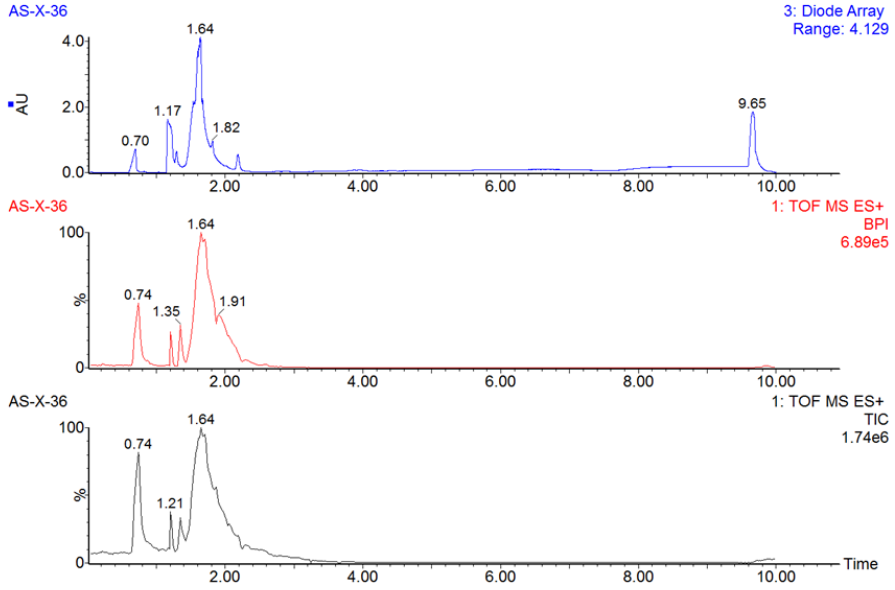
AS-X-36 98 (1.739)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
467.9703	467.9711	-0.8	-1.7	14.5	276.5	0.006	99.37	C21 H16 N3 Br2
	467.9722	-1.9	-4.1	-0.5	281.6	5.068	0.63	C9 H25 N7 Br3



$[M+H]^+$: $C_{21}H_{16}N_3Br$
Exact Mass: 467.9711



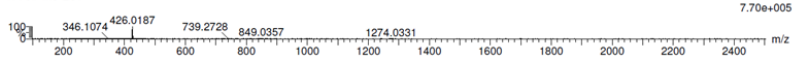
Compound 4x

Elemental Composition Report

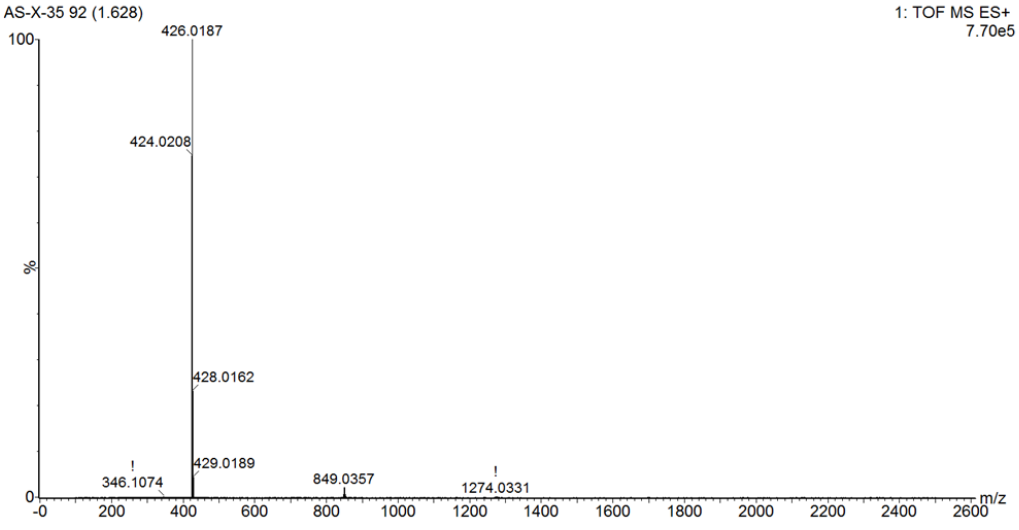
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

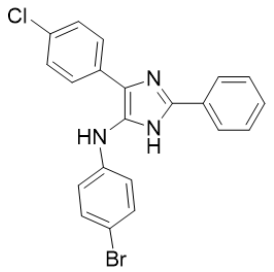
Monoisotopic Mass, Even Electron Ions
865 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Cl: 0-8 Br: 0-8

AS-X-35 92 (1.628)
1: TOF MS ES+
7.70e+005

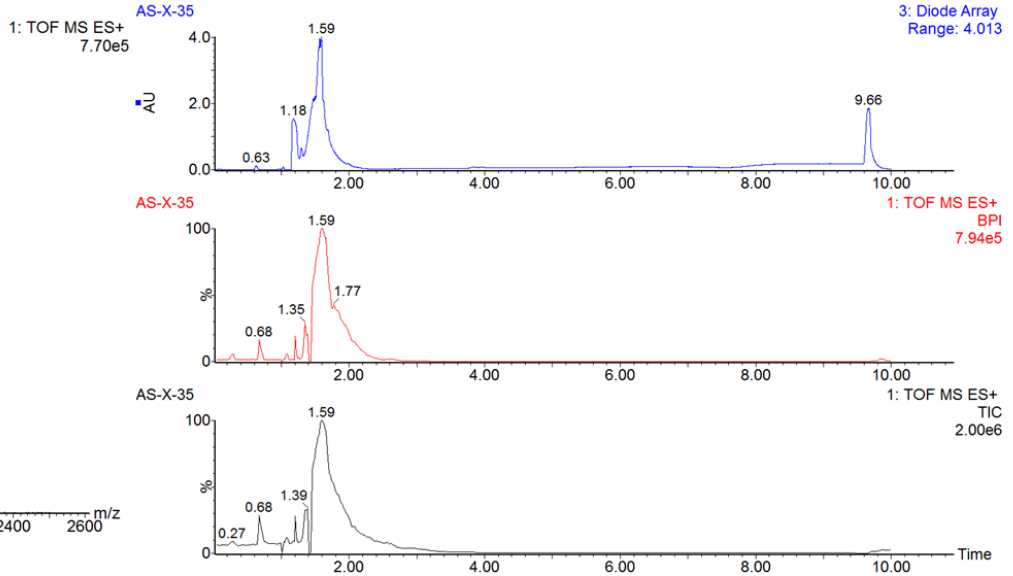


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
424.0208	424.0216	-0.8	-1.9	14.5	479.2	0.191	82.60	C21 H16 N3 Cl Br
	424.0193	1.5	3.5	11.5	480.9	1.857	15.61	C21 H18 N Cl4
	424.0234	-2.6	-6.1	9.5	484.1	5.034	0.65	C20 H21 N Cl2 Br
	424.0198	1.0	2.4	19.5	484.2	5.146	0.58	C22 H11 N5 Br
	424.0208	0.0	0.0	4.5	485.3	6.296	0.18	C10 H20 N9 Br2
	424.0167	4.1	9.7	6.5	485.5	6.465	0.16	C11 H17 N9 Cl2 Br
	424.0186	2.2	5.2	1.5	485.8	6.797	0.11	C10 H22 N7 Cl3 Br
	424.0227	-1.9	-4.5	-0.5	486.4	7.384	0.06	C9 H25 N7 Cl Br2
	424.0175	3.3	7.8	16.5	487.1	8.033	0.03	C22 H13 N3 Cl3
	424.0163	4.5	10.6	-1.5	488.5	9.422	0.01	C10 H24 N5 C16
	424.0187	2.1	5.0	34.5	500.3	21.250	0.00	C34 H2 N





$[M+H]^+$: $C_{21}H_{16}N_3ClBr$
Exact Mass: 424.0216



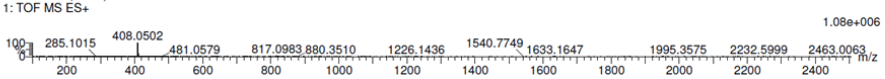
Compound 4y

Elemental Composition Report

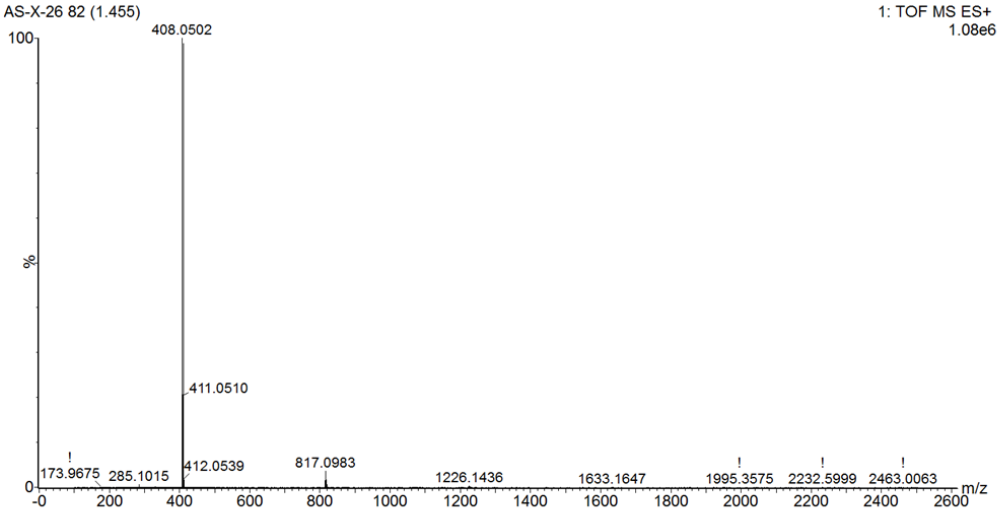
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

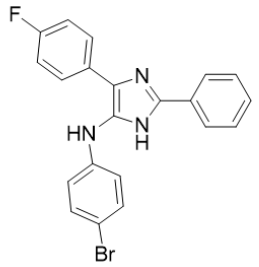
Monoisotopic Mass, Even Electron Ions
1178 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8 F: 0-10

AS-X-26 82 (1.455)
1: TOF MS ES+

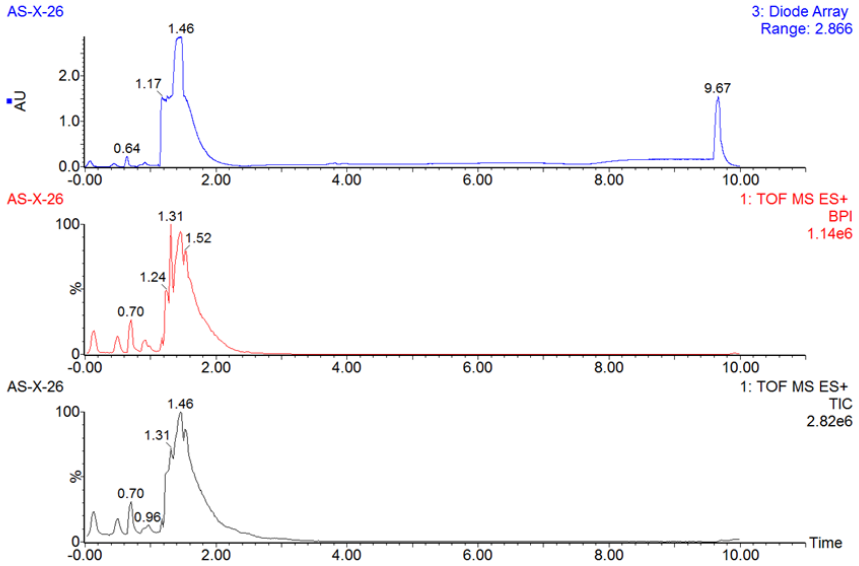


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.0502	408.0512	-1.0	-2.5	14.5	573.8	0.160	85.23	C21 H16 N3 Br F
	408.0510	-0.8	-2.0	3.5	575.9	2.162	11.51	C13 H17 N3 Br F6
	408.0508	-0.6	-1.5	7.5	577.1	3.423	3.26	C11 H14 N9 Br F3
	408.0522	-2.0	-4.9	-0.5	583.4	9.717	0.01	C9 H25 N7 Br2 F
	408.0462	4.0	9.8	-0.5	584.4	10.684	0.00	C12 H26 N3 Br2 F2
	408.0495	0.7	1.7	11.5	594.9	21.199	0.00	C15 H6 N5 F8
	408.0497	0.5	1.2	22.5	595.0	21.316	0.00	C23 H5 N5 F3





$[M+H]^+$: $C_{21}H_{16}N_3BrF$
Exact Mass: 408.0512



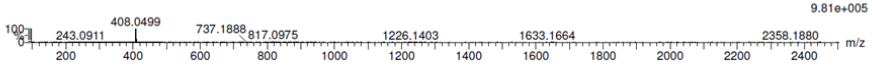
Compound 4z

Elemental Composition Report

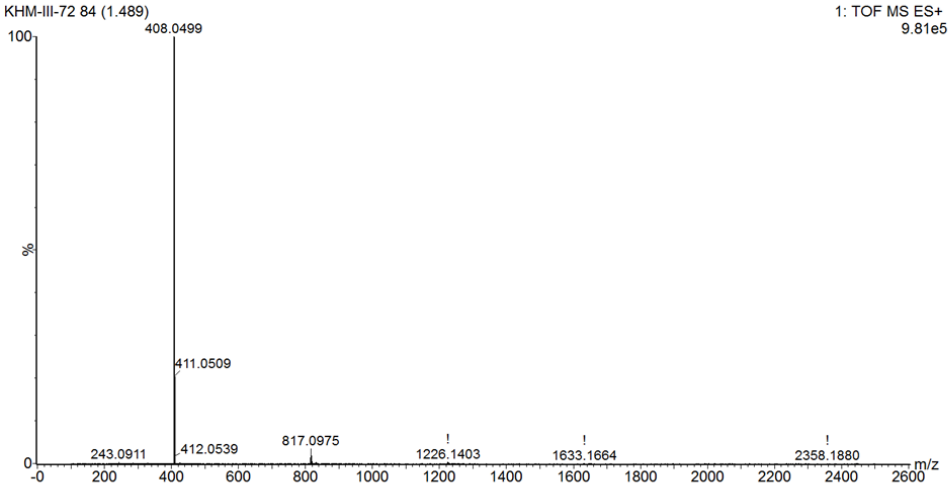
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

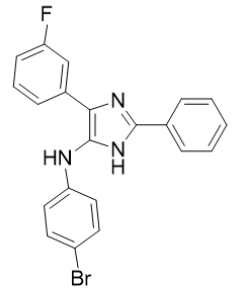
Monoisotopic Mass, Even Electron Ions
1178 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8 F: 0-10

KHM-III-72 84 (1.489)
1: TOF MS ES+
9.81e+005

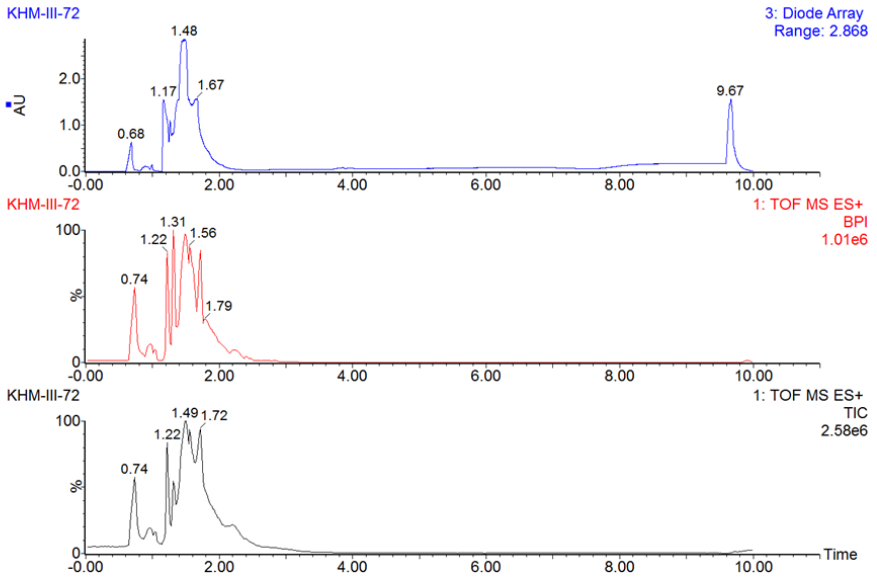


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.0499	408.0512	-1.3	-3.2	14.5	472.5	0.162	85.04	C21 H16 N3 Br F
	408.0510	-1.1	-2.7	3.5	474.3	2.015	13.33	C13 H17 N3 Br F6
	408.0508	-0.9	-2.2	7.5	476.4	4.119	1.63	C11 H14 N9 Br F3
	408.0462	3.7	9.1	-0.5	482.5	10.207	0.00	C12 H26 N3 Br2 F2
	408.0522	-2.3	-5.6	-0.5	482.7	10.366	0.00	C9 H25 N7 Br2 F
	408.0495	0.4	1.0	11.5	493.5	21.216	0.00	C15 H6 N5 F8
	408.0497	0.2	0.5	22.5	493.7	21.327	0.00	C23 H5 N5 F3





$[M+H]^+$: $C_{21}H_{16}N_3BrF$
Exact Mass: 408.0512



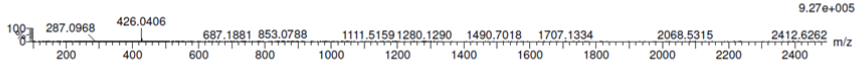
Compound 4aa

Elemental Composition Report

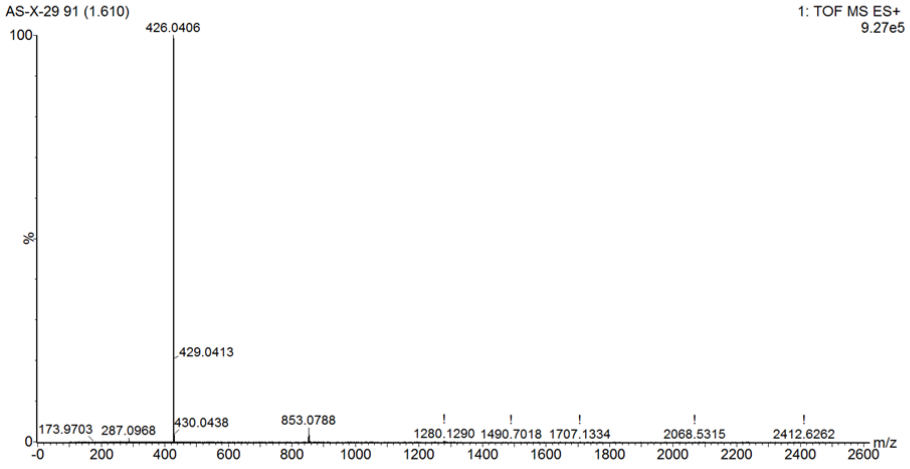
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

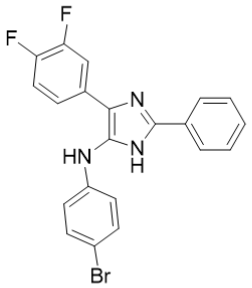
Monoisotopic Mass, Even Electron Ions
1295 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8 F: 0-10

AS-X-29 91 (1.610)
1: TOF MS ES+

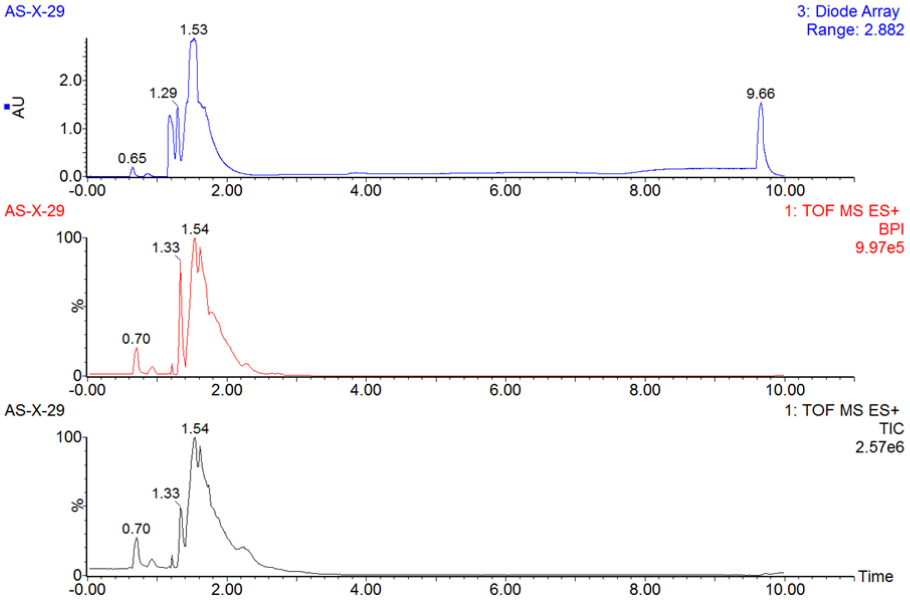


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
426.0406	426.0417	-1.1	-2.6	14.5	528.9	0.090	91.39	C21 H15 N3 Br F2
	426.0416	-1.0	-2.3	3.5	531.4	2.645	7.10	C13 H16 N3 Br F7
	426.0413	-0.7	-1.6	7.5	533.0	4.199	1.50	C11 H13 N9 Br F4
	426.0432	-2.6	-6.1	6.5	538.5	9.757	0.01	C19 H26 N Br2
	426.0428	-2.2	-5.2	-0.5	539.1	10.367	0.00	C9 H24 N7 Br2 F2
	426.0367	3.9	9.2	-0.5	539.6	10.817	0.00	C12 H25 N3 Br2 F3
	426.0365	4.1	9.6	3.5	540.9	12.164	0.00	C10 H22 N9 Br2
	426.0401	0.5	1.2	11.5	550.2	21.395	0.00	C15 H5 N5 F9
	426.0403	0.3	0.7	22.5	550.3	21.505	0.00	C23 H4 N5 F4





$[M+H]^+$: $C_{21}H_{15}N_3BrF_2$
Exact Mass: 426.0417



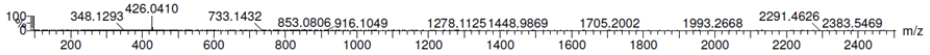
Compound 4ab

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

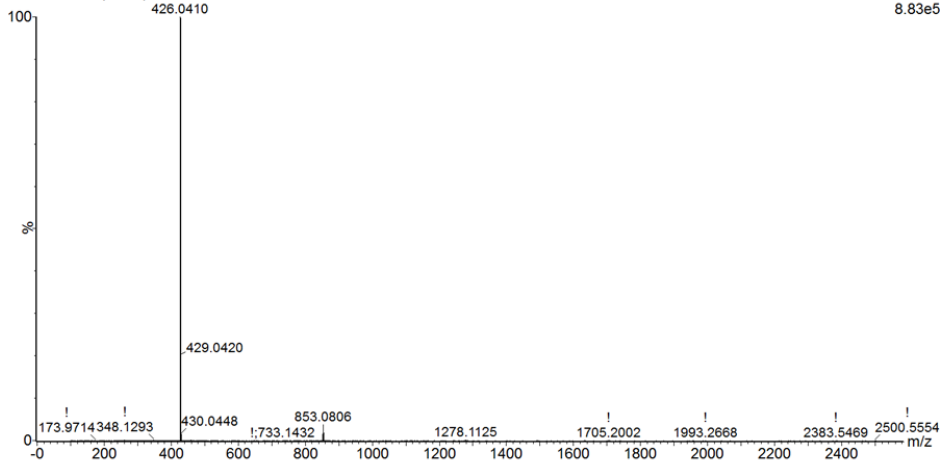
Monoisotopic Mass, Even Electron Ions
1295 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10 Br: 0-8

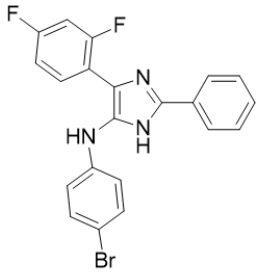
KHM-III-84 82 (1.455)
1: TOF MS ES+
8.83e+005



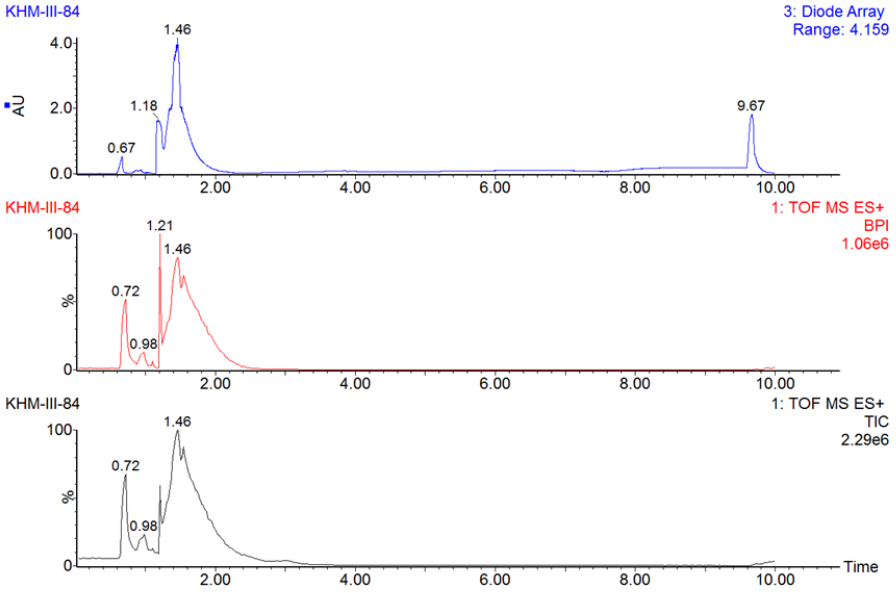
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
426.0410	426.0417	-0.7	-1.6	14.5	543.6	0.045	95.55	C21 H15 N3 F2 Br
	426.0416	-0.6	-1.4	3.5	546.7	3.182	4.15	C13 H16 N3 F7 Br
	426.0413	-0.3	-0.7	7.5	549.4	5.857	0.29	C11 H13 N9 F4 Br
	426.0432	-2.2	-5.2	6.5	552.8	9.296	0.01	C19 H26 N Br2
	426.0428	-1.8	-4.2	-0.5	555.1	11.608	0.00	C9 H24 N7 F2 Br2
	426.0367	4.3	10.1	-0.5	555.3	11.762	0.00	C12 H25 N3 F3 Br2
	426.0365	4.5	10.6	3.5	556.9	13.339	0.00	C10 H22 N9 Br2
	426.0401	0.9	2.1	11.5	565.3	21.774	0.00	C15 H5 N5 F9
	426.0403	0.7	1.6	22.5	565.4	21.873	0.00	C23 H4 N5 F4

KHM-III-84 82 (1.455)
1: TOF MS ES+
8.83e5





$[M+H]^+$: $C_{21}H_{15}N_3BrF_2$
Exact Mass: 426.0417



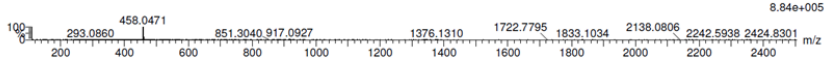
Compound 4ac

Elemental Composition Report

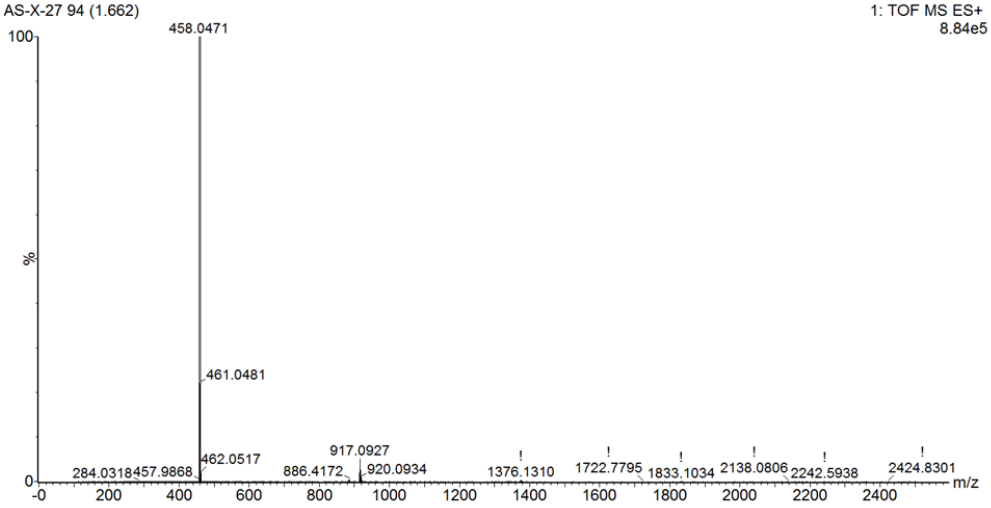
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

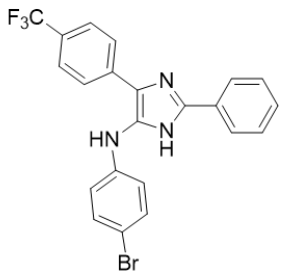
Monoisotopic Mass, Even Electron Ions
1528 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10 Br: 0-8

AS-X-27 94 (1.662)
1: TOF MS ES+
8.84e+005

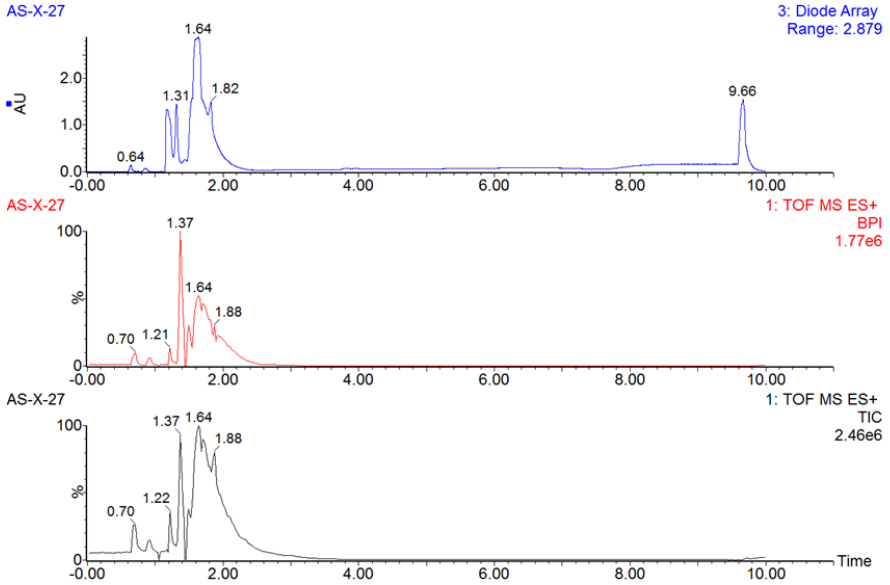


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
458.0471	458.0477	-0.6	-1.3	18.5	539.4	0.708	49.25	C20 H13 N9 Br
	458.0480	-0.9	-2.0	14.5	539.4	0.763	46.62	C22 H16 N3 F3 Br
	458.0478	-0.7	-1.5	3.5	542.2	3.564	2.83	C14 H17 N3 F8 Br
	458.0476	-0.5	-1.1	7.5	543.0	4.348	1.29	C12 H14 N9 F5 Br
	458.0490	-1.9	-4.1	-0.5	549.3	10.593	0.00	C10 H25 N7 F3 Br2
	458.0494	-2.3	-5.0	6.5	549.4	10.684	0.00	C20 H27 N F Br2
	458.0430	4.1	9.0	-0.5	550.8	12.147	0.00	C13 H26 N3 F4 Br2
	458.0427	4.4	9.6	3.5	551.6	12.962	0.00	C11 H23 N9 F Br2
	458.0464	0.7	1.5	11.5	560.6	21.942	0.00	C16 H6 N5 F10
	458.0465	0.6	1.3	22.5	560.7	22.033	0.00	C24 H5 N5 F5
	458.0467	0.4	0.9	33.5	560.8	22.128	0.00	C32 H4 N5





$[M+H]^+$: $C_{22}H_{16}N_3F_3Br$
Exact Mass: 458.0480



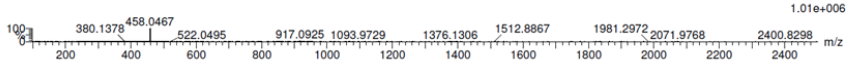
Compound 4ad

Elemental Composition Report

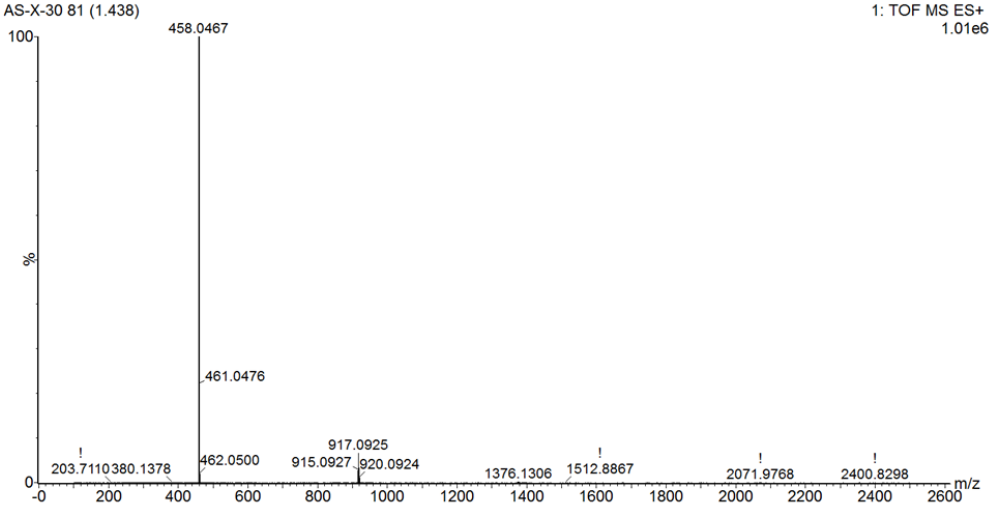
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

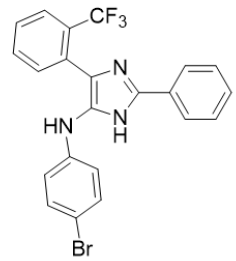
Monoisotopic Mass, Even Electron Ions
1528 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10 Br: 0-8

AS-X-30 81 (1.438)
1: TOF MS ES+

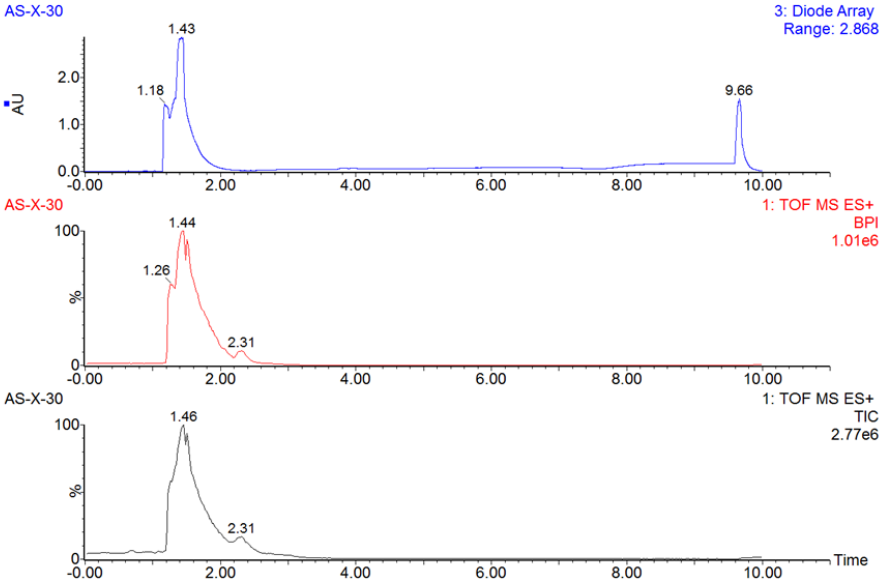


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
458.0467	458.0480	-1.3	-2.8	14.5	507.1	0.723	48.51	C22 H16 N3 F3 Br
	458.0477	-1.0	-2.2	18.5	507.1	0.734	48.01	C20 H13 N9 Br
	458.0478	-1.1	-2.4	3.5	510.1	3.700	2.47	C14 H17 N3 F8 Br
	458.0476	-0.9	-2.0	7.5	511.0	4.601	1.00	C12 H14 N9 F5 Br
	458.0494	-2.7	-5.9	6.5	517.3	10.894	0.00	C20 H27 N F Br2
	458.0490	-2.3	-5.0	-0.5	517.3	10.920	0.00	C10 H25 N7 F3 Br2
	458.0430	3.7	8.1	-0.5	518.1	11.729	0.00	C13 H26 N3 F4 Br2
	458.0427	4.0	8.7	3.5	519.2	12.765	0.00	C11 H23 N9 F Br2
	458.0464	0.3	0.7	11.5	528.5	22.060	0.00	C16 H6 N5 F10
	458.0465	0.2	0.4	22.5	528.6	22.147	0.00	C24 H5 N5 F5
	458.0467	0.0	0.0	33.5	528.7	22.239	0.00	C32 H4 N5





$[M+H]^+$: $C_{22}H_{16}N_3F_3Br$
Exact Mass: 458.0480



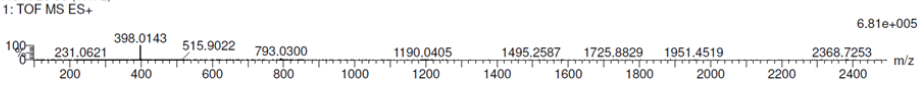
Compound 4ae

Elemental Composition Report

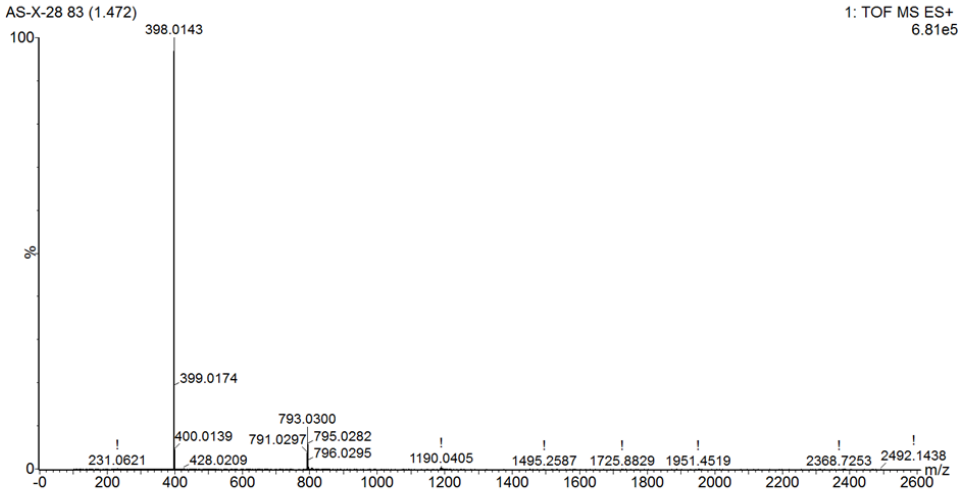
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

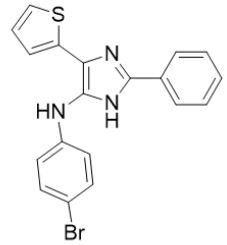
Monoisotopic Mass, Even Electron Ions
448 formula(e) evaluated with 6 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 S: 0-2 Br: 0-8

AS-X-28 83 (1.472)
1: TOF MS ES+

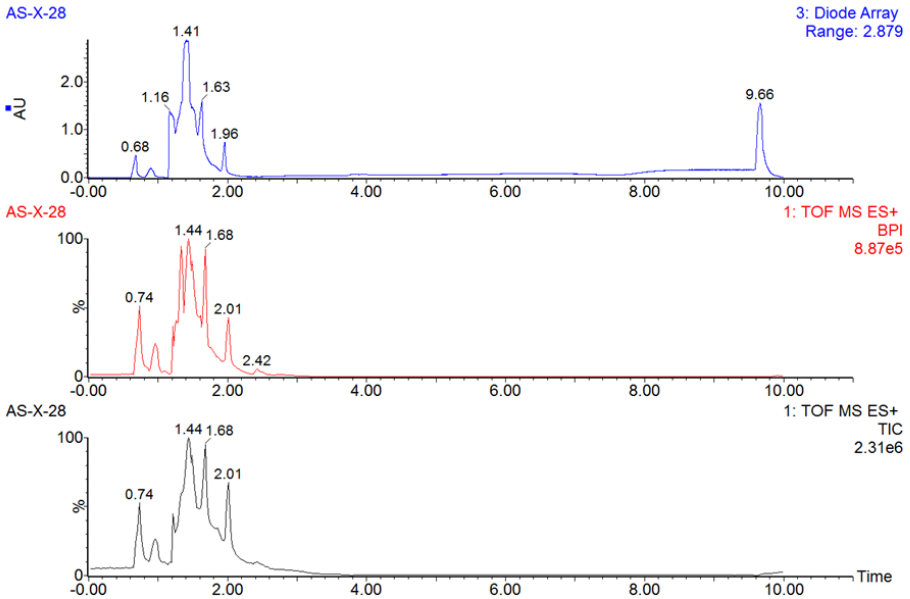


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
396.0164	396.0204	-4.0	-10.1	8.5	481.7	0.595	55.15	C16 H19 N3 S2 Br
	396.0170	-0.6	-1.5	13.5	481.9	0.821	43.98	C19 H15 N3 S Br
	396.0136	2.8	7.1	18.5	485.8	4.750	0.87	C22 H11 N3 Br
	396.0147	1.7	4.3	3.5	491.5	10.453	0.00	C10 H20 N7 Br2
	396.0181	-1.7	-4.3	-1.5	493.1	12.027	0.00	C7 H24 N7 S Br2
	396.0126	3.8	9.6	20.5	495.2	14.128	0.00	C19 H6 N7 S2





$[M+H]^+$: $C_{19}H_{15}N_3SBr$
Exact Mass: 396.0170



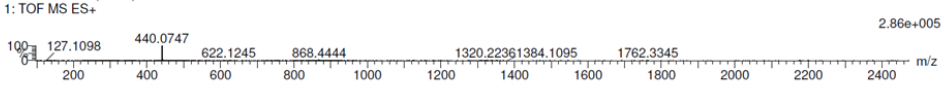
Compound 4af

Elemental Composition Report

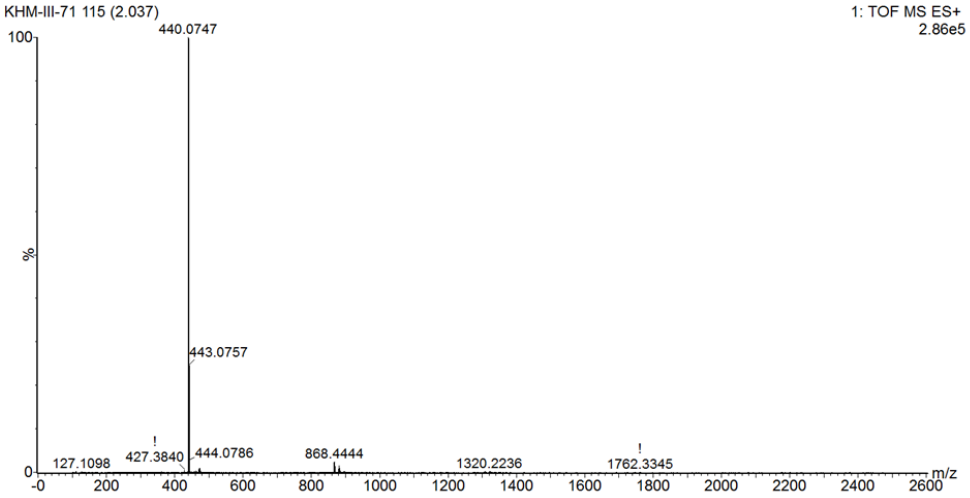
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

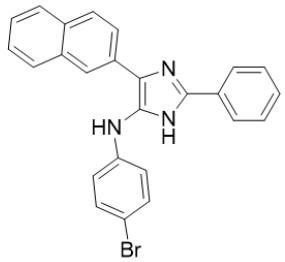
Monoisotopic Mass, Even Electron Ions
208 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

KHM-III-71 115 (2.037)
1: TOF MS ES+

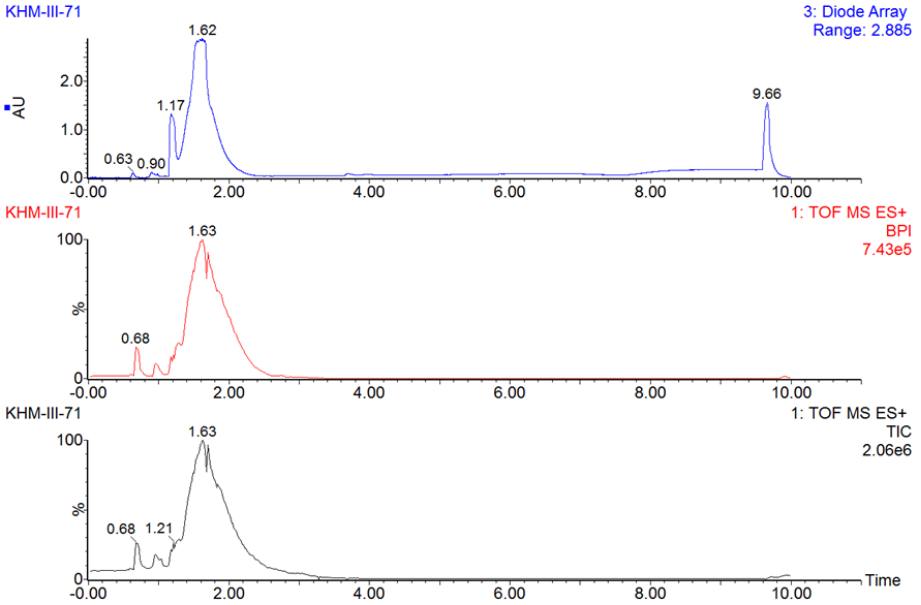


	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
440.0747	440.0762	-1.5	-3.4	17.5	331.0	0.000	99.99	C25 H19 N3 Br
	440.0773	-2.6	-5.9	2.5	340.7	9.726	0.01	C13 H28 N7 Br2





$[M+H]^+$: $C_{25}H_{19}N_3Br$
Exact Mass: 440.0762



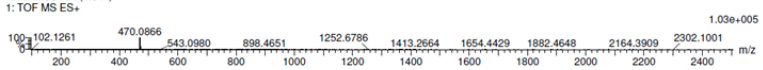
Compound 4ag

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

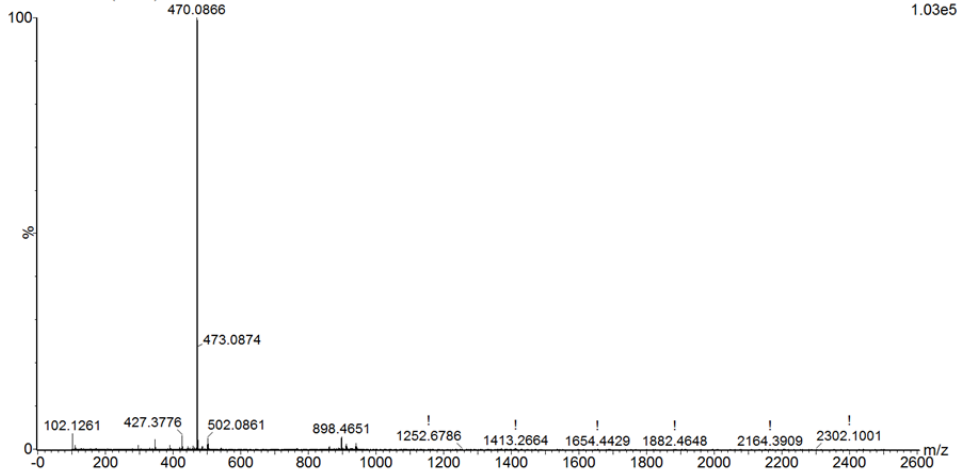
Monoisotopic Mass, Even Electron Ions
2519 formula(e) evaluated with 19 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

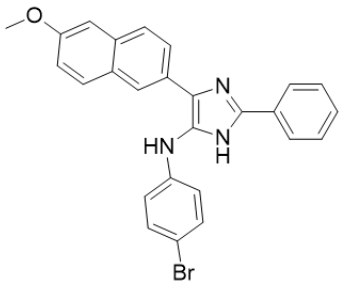
KHM-III-86 104 (1.841)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
470.0866	470.0828	3.8	8.1	13.5	225.6	0.033	96.76	C21 H21 N5 O3 Br
	470.0868	-0.2	-0.4	17.5	229.6	4.028	1.78	C26 H21 N3 O Br
	470.0900	-3.4	-7.2	9.5	230.3	4.734	0.88	C15 H21 N9 O4 Br
	470.0887	-2.1	-4.5	4.5	231.0	5.429	0.44	C14 H25 N5 O8 Br
	470.0873	-0.7	-1.5	-0.5	232.3	6.683	0.13	C13 H29 N O12 Br
	470.0846	2.0	4.3	0.5	234.2	8.641	0.02	C9 H25 N7 O10 Br
	470.0879	-1.3	-2.8	2.5	236.5	10.945	0.00	C14 H30 N7 O Br2
	470.0905	-3.9	-8.3	1.5	238.7	13.164	0.00	C18 H34 N O3 Br2
	470.0838	2.8	6.0	-1.5	239.1	13.485	0.00	C9 H30 N9 O3 Br2
	470.0854	1.2	2.6	2.5	247.5	21.958	0.00	C9 H20 N5 O17
	470.0868	-0.2	-0.4	7.5	247.6	22.005	0.00	C10 H16 N9 O13
	470.0894	-2.8	-6.0	6.5	247.7	22.078	0.00	C14 H20 N3 O15
	470.0908	-4.2	-8.9	11.5	247.7	22.160	0.00	C15 H16 N7 O11
	470.0849	1.7	3.6	20.5	247.9	22.268	0.00	C22 H12 N7 O6
	470.0836	3.0	6.4	15.5	247.9	22.276	0.00	C21 H16 N3 O10
	470.0876	-1.0	-2.1	19.5	248.1	22.551	0.00	C26 H16 N O8
	470.0903	-3.7	-7.9	29.5	248.2	22.594	0.00	C28 H8 N9
	470.0889	-2.3	-4.9	24.5	248.2	22.597	0.00	C27 H12 N5 O4
	470.0817	4.9	10.4	28.5	248.4	22.831	0.00	C33 H12 N O3

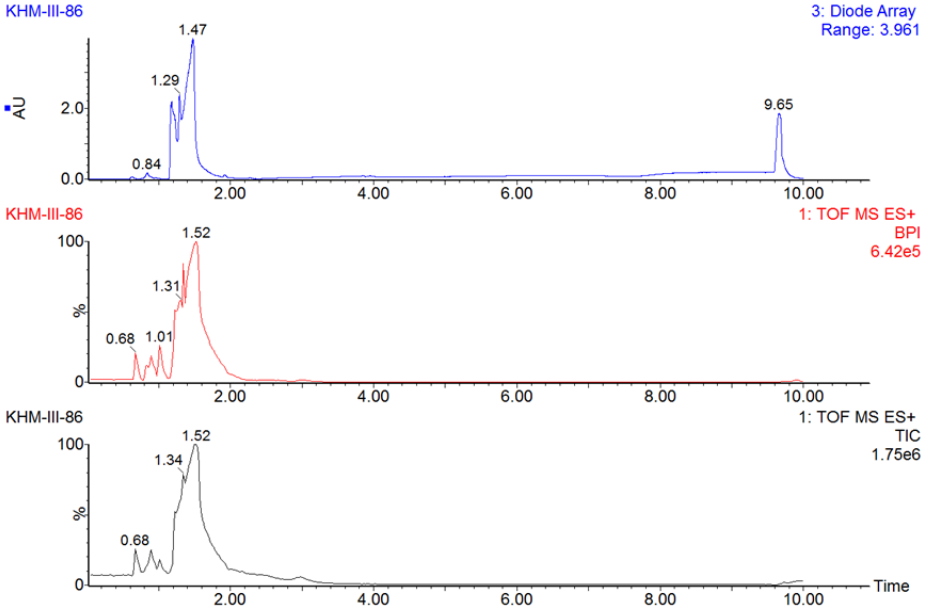
KHM-III-86 104 (1.841)





$[M+H]^+$: $C_{26}H_{20}N_3OBr$
Exact Mass: 470.0868

1: TOF MS ES+
1.03e5



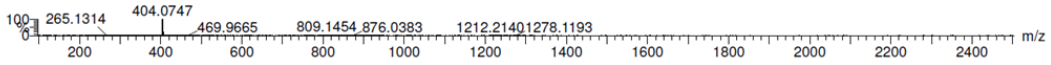
Compound 4ah

Elemental Composition Report

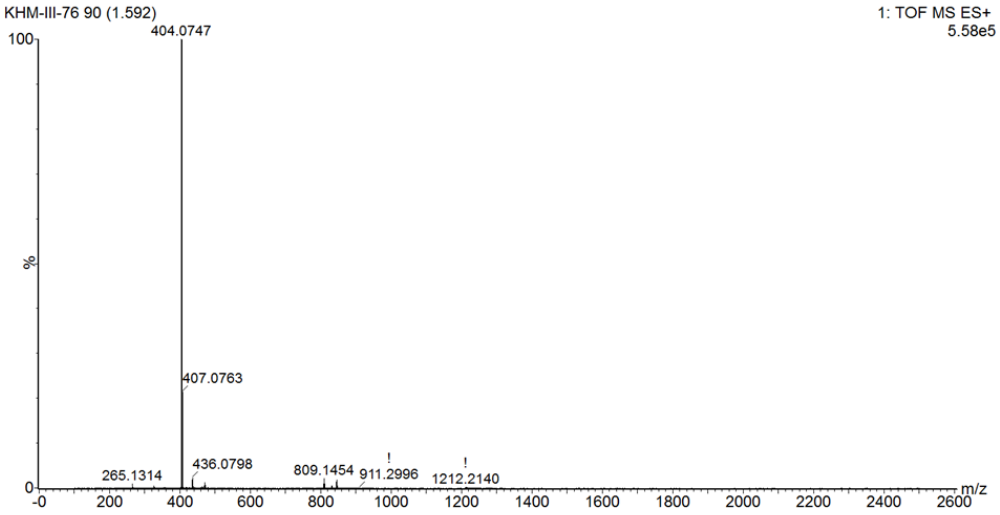
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

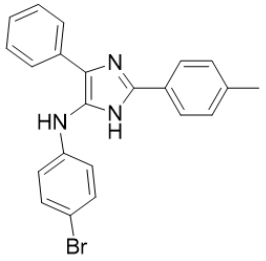
Monoisotopic Mass, Even Electron Ions
179 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

KHM-III-76 90 (1.592)
1: TOF MS ES+

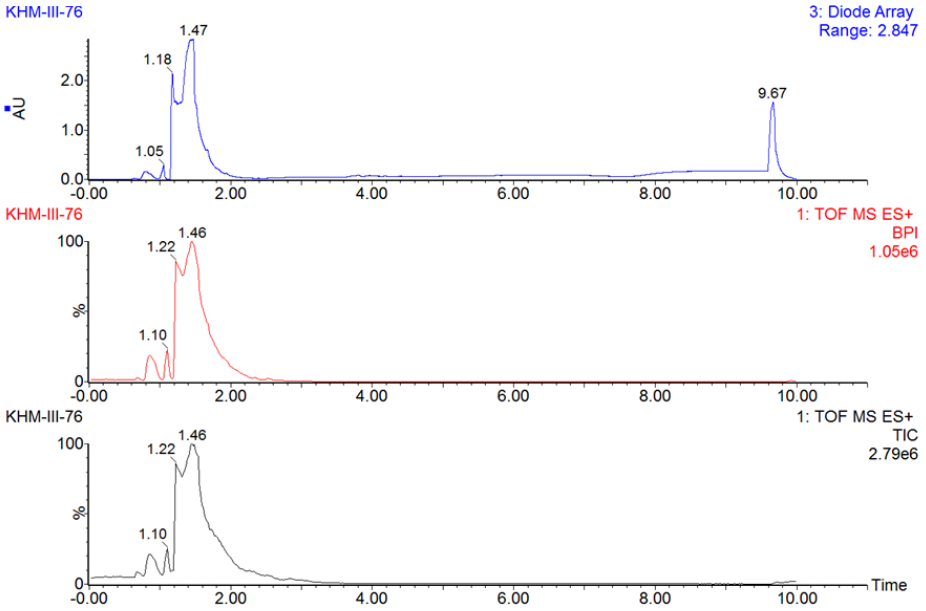


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
404.0747	404.0762	-1.5	-3.7	14.5	445.9	0.000	100.00	C22 H19 N3 Br
	404.0773	-2.6	-6.4	-0.5	456.5	10.553	0.00	C10 H28 N7 Br2





$[M+H]^+$: $C_{22}H_{19}N_3Br$
Exact Mass: 404.0762



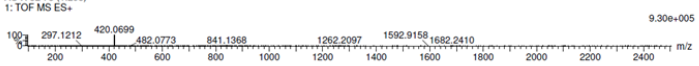
Compound 4ai

Elemental Composition Report

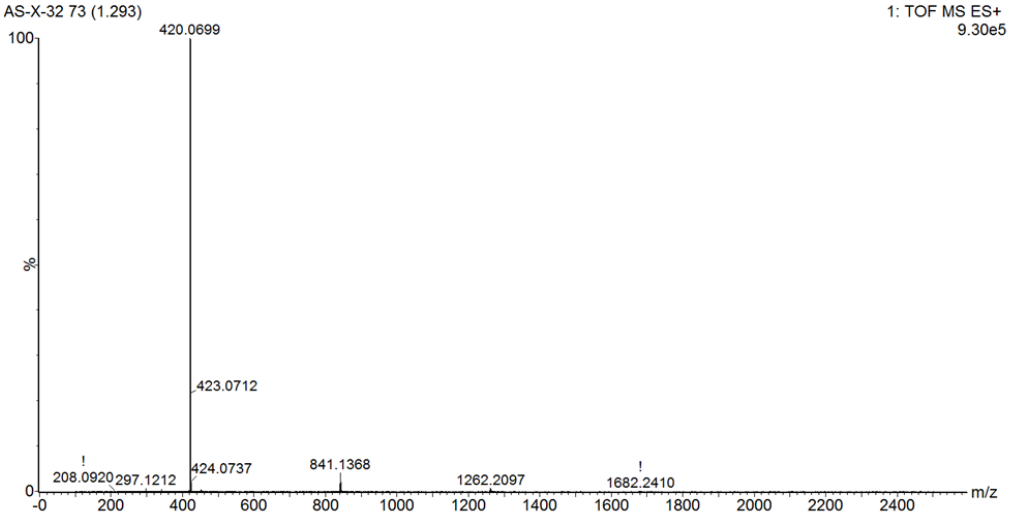
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

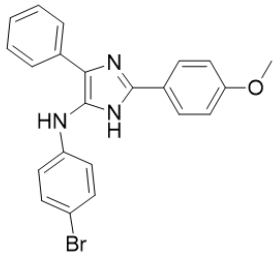
Monoisotopic Mass, Even Electron Ions
1896 formula(e) evaluated with 18 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

AS-X-32 73 (1.293)
1: TOF MS ES+

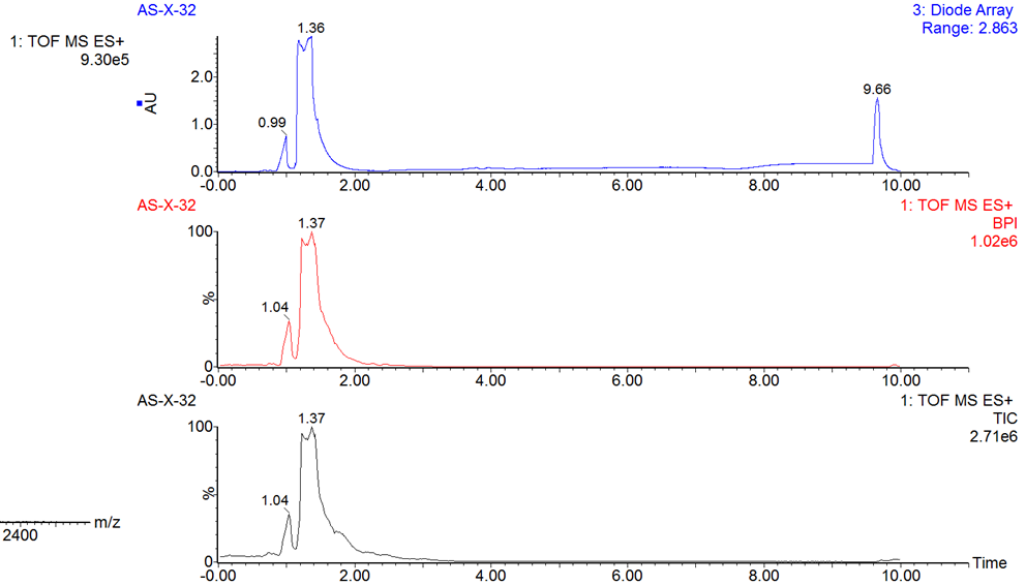


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
420.0699	420.0671	2.8	6.7	10.5	556.8	0.073	92.92	C17 H19 N5 O3 Br
	420.0712	-1.3	-3.1	14.5	559.5	2.708	6.67	C22 H19 N3 O Br
	420.0658	4.1	9.8	5.5	562.4	5.616	0.36	C16 H23 N O7 Br
	420.0730	-3.1	-7.4	1.5	564.9	8.150	0.03	C10 H23 N5 O8 Br
	420.0743	-4.4	-10.5	6.5	565.3	8.490	0.02	C11 H19 N9 O4 Br
	420.0722	-2.3	-5.5	-0.5	569.1	12.277	0.00	C10 H28 N7 O Br2
	420.0650	4.9	11.7	3.5	570.6	13.821	0.00	C16 H28 N3 Br2
	420.0749	-5.0	-11.9	-1.5	571.0	14.269	0.00	C14 H32 N O3 Br2
	420.0652	4.7	11.2	13.5	579.9	23.108	0.00	C13 H10 N9 O8
	420.0738	-3.9	-9.3	3.5	579.9	23.133	0.00	C10 H18 N3 O15
	420.0698	0.1	0.2	-0.5	580.0	23.240	0.00	C5 H18 N5 O17
	420.0679	2.0	4.8	12.5	580.0	23.251	0.00	C17 H14 N3 O10
	420.0693	0.6	1.4	17.5	580.0	23.275	0.00	C18 H10 N7 O6
	420.0711	-1.2	-2.9	4.5	580.1	23.303	0.00	C6 H14 N9 O13
	420.0719	-2.0	-4.8	16.5	580.3	23.553	0.00	C22 H14 N O8
	420.0733	-3.4	-8.1	21.5	580.4	23.603	0.00	C23 H10 N5 O4
	420.0746	-4.7	-11.2	26.5	580.4	23.614	0.00	C24 H6 N9
	420.0661	3.8	9.0	25.5	580.6	23.861	0.00	C29 H10 N O3





$[M+H]^+$: $C_{22}H_{19}N_3OBr$
Exact Mass: 420.0712



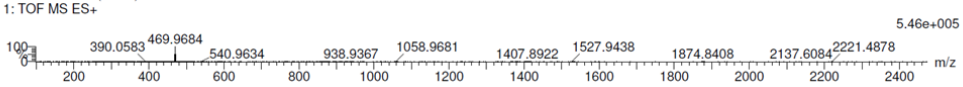
Compound 4aj

Elemental Composition Report

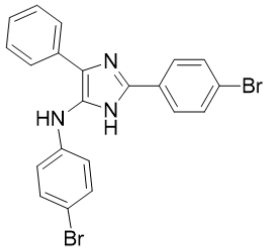
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
232 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

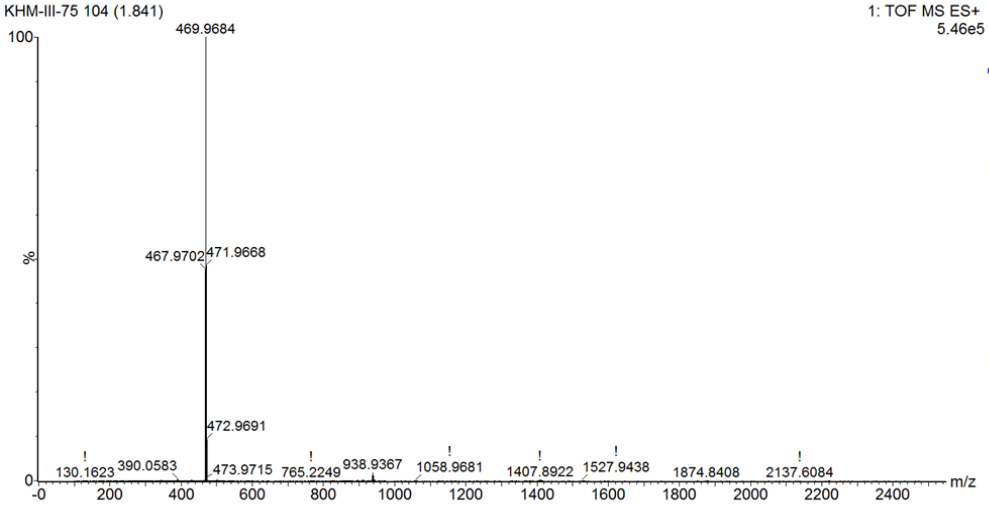
KHM-III-75 104 (1.841)
1: TOF MS ES+

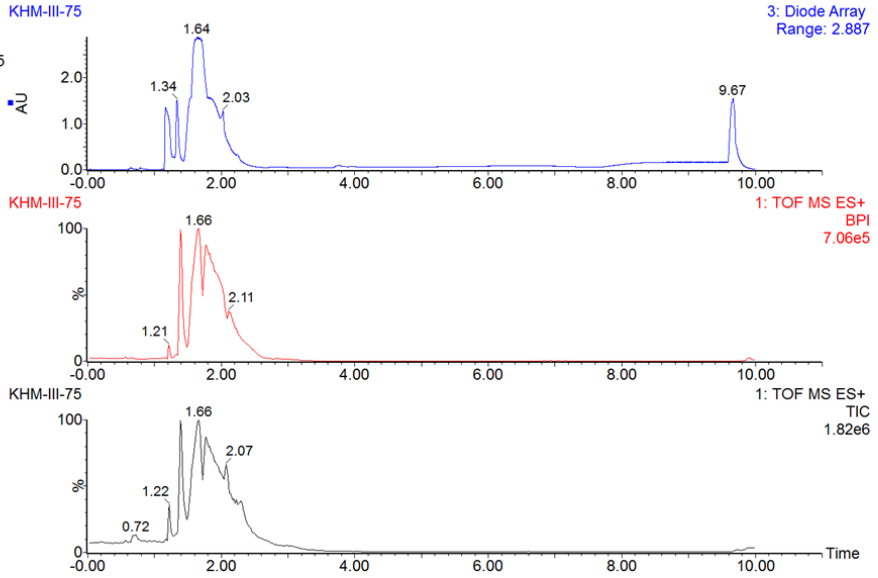


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
467.9702	467.9711	-0.9	-1.9	14.5	390.4	0.001	99.92	C21 H16 N3 Br2
	467.9722	-2.0	-4.3	-0.5	397.5	7.163	0.08	C9 H25 N7 Br3



$[M+H]^+$: $C_{21}H_{16}N_3Br_2$
Exact Mass: 467.9711





Compound 4ak

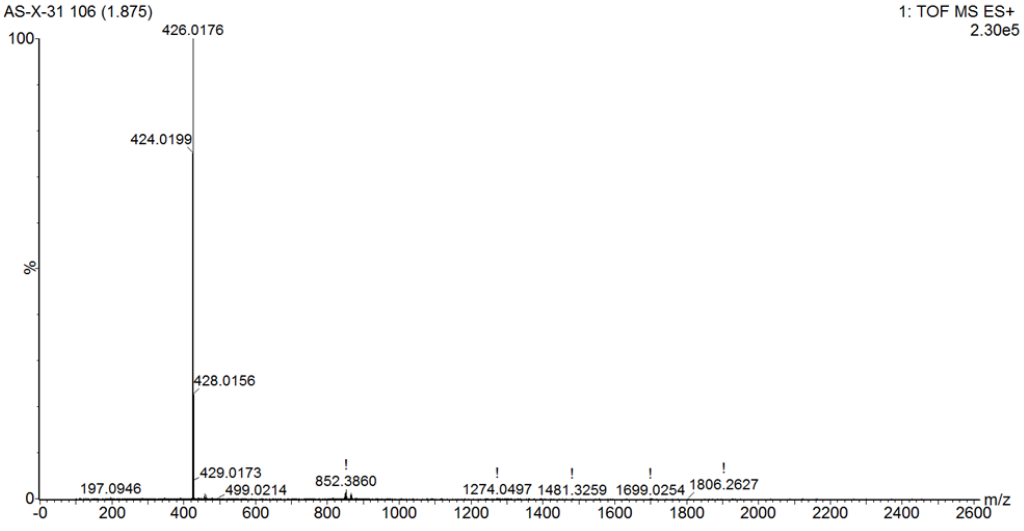
Elemental Composition Report

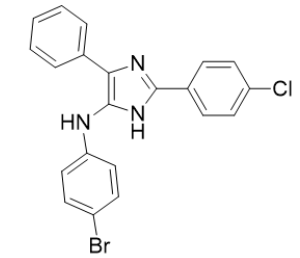
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
865 formula(e) evaluated with 12 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Cl: 0-8 Br: 0-8

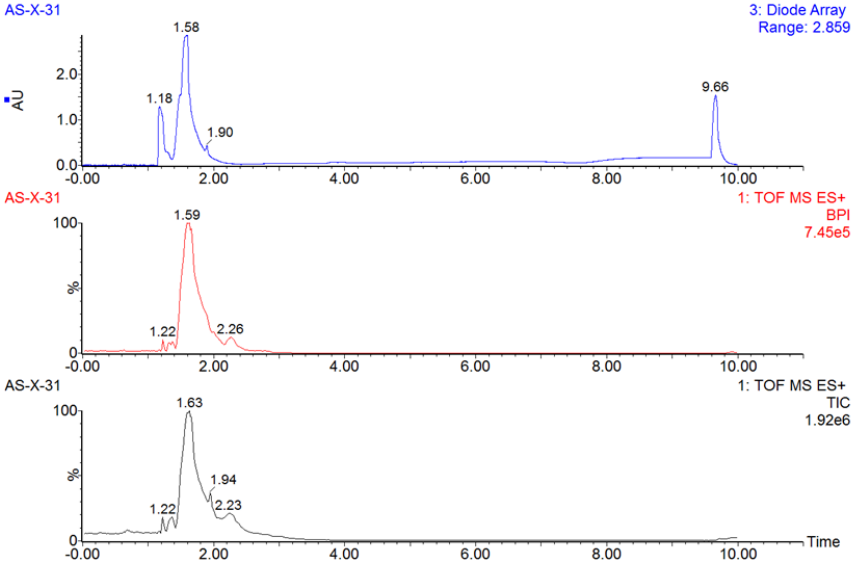
AS-X-31 106 (1.875)
1: TOF MS ES+
2.30e+005

Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
424.0199	424.0193	0.6	1.4	11.5	265.3	0.382	68.24	C21 H18 N Cl4
	424.0216	-1.7	-4.0	14.5	266.1	1.248	28.70	C21 H16 N3 Cl Br
	424.0234	-3.5	-8.3	9.5	268.6	3.756	2.34	C20 H21 N Cl2 Br
	424.0175	2.4	5.7	16.5	270.8	5.912	0.27	C22 H13 N3 Cl3
	424.0198	0.1	0.2	19.5	270.9	6.031	0.24	C22 H11 N5 Br
	424.0167	3.2	7.5	6.5	271.6	6.764	0.12	C11 H17 N9 Cl2 Br
	424.0186	1.3	3.1	1.5	272.6	7.703	0.05	C10 H22 N7 Cl3 Br
	424.0163	3.6	8.5	-1.5	273.1	8.251	0.03	C10 H24 N5 Cl6
	424.0208	-0.9	-2.1	4.5	273.7	8.825	0.01	C10 H20 N9 Br2
	424.0227	-2.8	-6.6	-0.5	274.5	9.662	0.01	C9 H25 N7 Cl Br2
	424.0157	4.2	9.9	21.5	275.0	10.107	0.00	C23 H8 N5 Cl2
	424.0187	1.2	2.8	34.5	285.9	21.045	0.00	C34 H2 N





$[M+H]^+$: $C_{21}H_{16}N_3ClBr$
Exact Mass: 424.0216



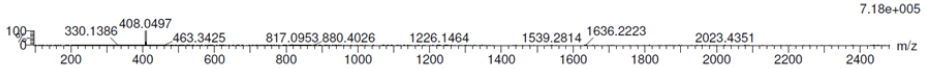
Compound 4al

Elemental Composition Report

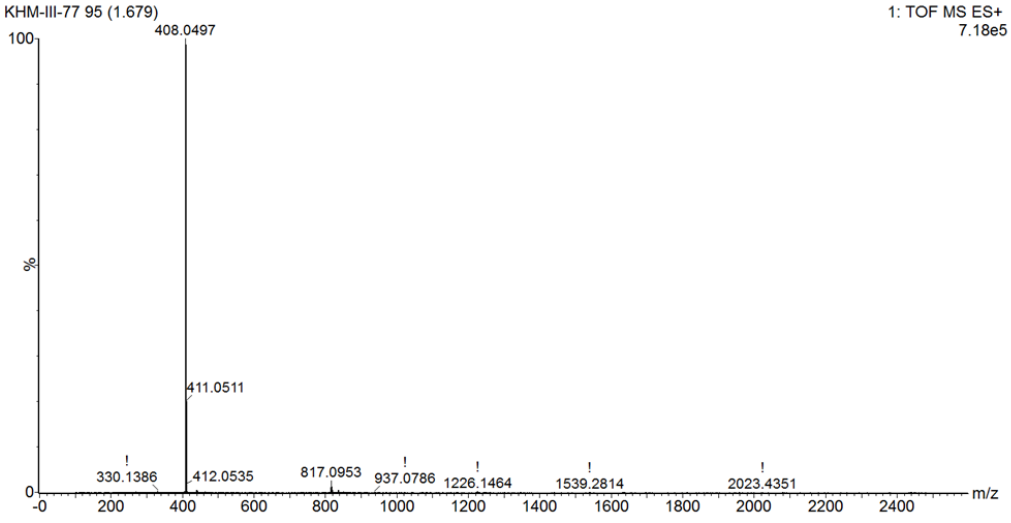
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

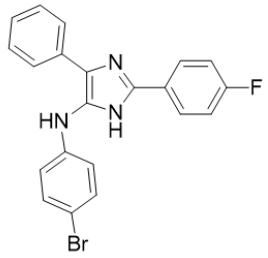
Monoisotopic Mass, Even Electron Ions
1178 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8 F: 0-10

KHM-III-77 95 (1.679)
1: TOF MS ES+

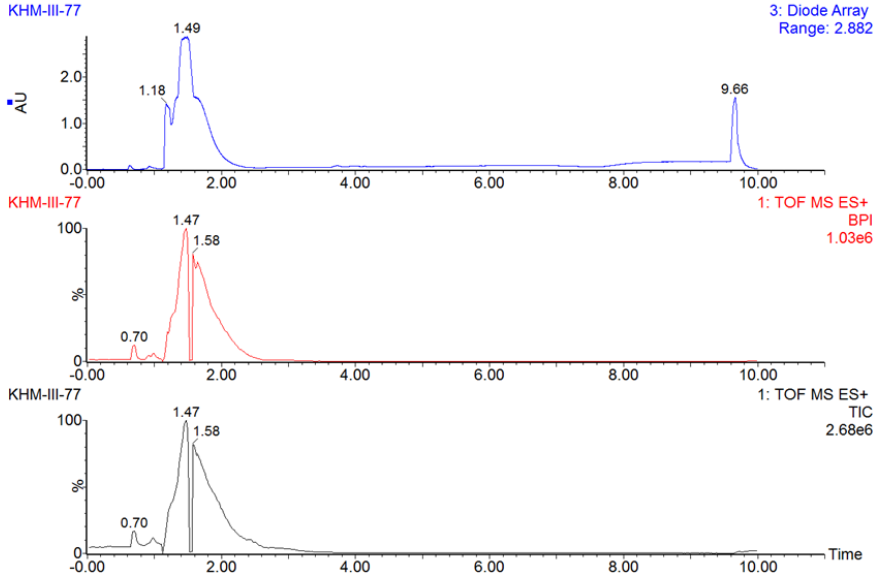


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
408.0497	408.0512	-1.5	-3.7	14.5	516.2	0.115	89.16	C21 H16 N3 Br F
	408.0510	-1.3	-3.2	3.5	518.6	2.455	8.59	C13 H17 N3 Br F6
	408.0508	-1.1	-2.7	7.5	519.9	3.795	2.25	C11 H14 N9 Br F3
	408.0522	-2.5	-6.1	-0.5	526.3	10.168	0.00	C9 H25 N7 Br2 F
	408.0462	3.5	8.6	-0.5	526.4	10.325	0.00	C12 H26 N3 Br2 F2
	408.0495	0.2	0.5	11.5	537.3	21.185	0.00	C15 H6 N5 F8
	408.0497	0.0	0.0	22.5	537.4	21.300	0.00	C23 H5 N5 F3





$[M+H]^+$: $C_{21}H_{16}N_3FBr$
Exact Mass: 408.0512



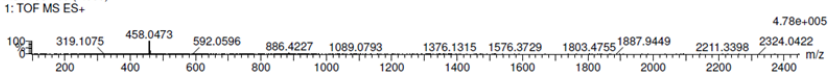
Compound 4am

Elemental Composition Report

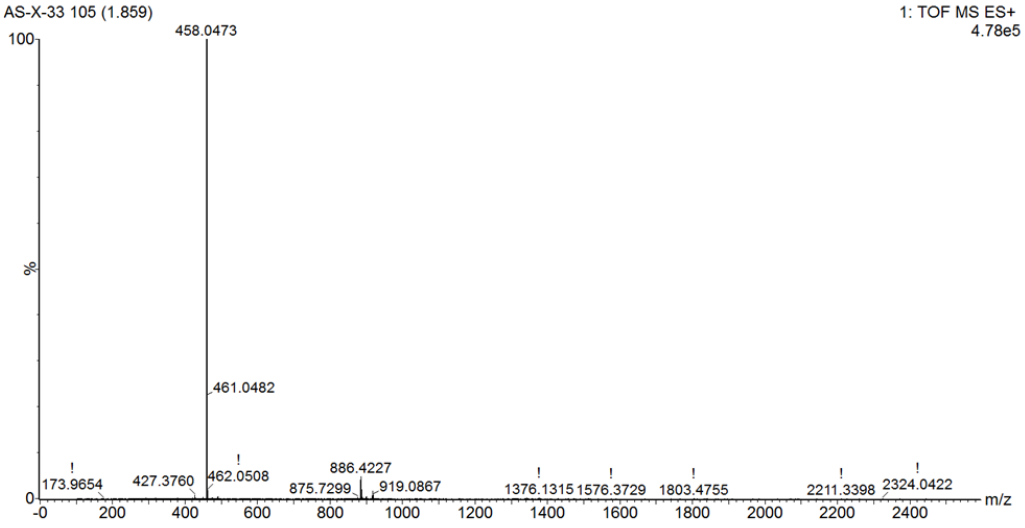
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

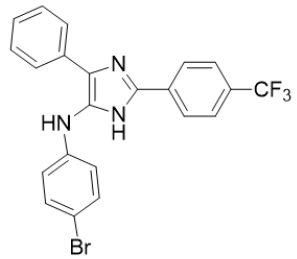
Monoisotopic Mass, Even Electron Ions
1528 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8 F: 0-10

AS-X-33 105 (1.859)
1: TOF MS ES+
4.78e+005

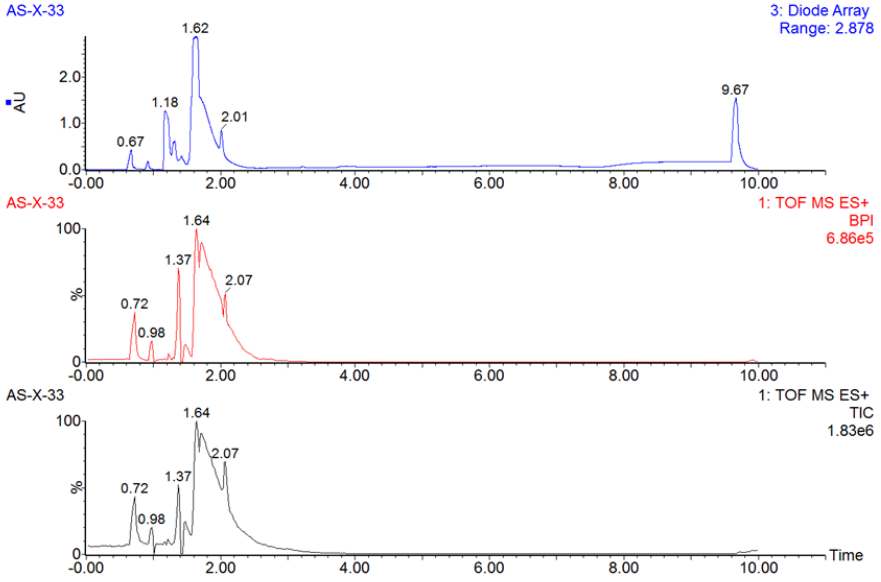


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
458.0473	458.0480	-0.7	-1.5	14.5	439.7	0.393	67.47	C22 H16 N3 Br F3
	458.0477	-0.4	-0.9	18.5	440.8	1.464	23.14	C20 H13 N9 Br
	458.0478	-0.5	-1.1	3.5	441.8	2.473	8.43	C14 H17 N3 Br F8
	458.0476	-0.3	-0.7	7.5	444.0	4.660	0.95	C12 H14 N9 Br F5
	458.0494	-2.1	-4.6	6.5	448.4	9.061	0.01	C20 H27 N Br2 F
	458.0490	-1.7	-3.7	-0.5	450.1	10.747	0.00	C10 H25 N7 Br2 F3
	458.0430	4.3	9.4	-0.5	450.9	11.572	0.00	C13 H26 N3 Br2 F4
	458.0427	4.6	10.0	3.5	452.2	12.895	0.00	C11 H23 N9 Br2 F
	458.0464	0.9	2.0	11.5	460.7	21.368	0.00	C16 H6 N5 F10
	458.0465	0.8	1.7	22.5	460.8	21.454	0.00	C24 H5 N5 F5
	458.0467	0.6	1.3	33.5	460.9	21.550	0.00	C32 H4 N5





$[M+H]^+$: $C_{22}H_{16}N_3F_3Br$
Exact Mass: 458.0480



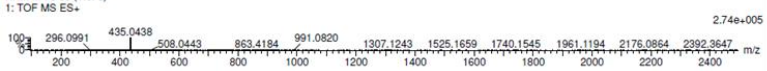
Compound 4an

Elemental Composition Report

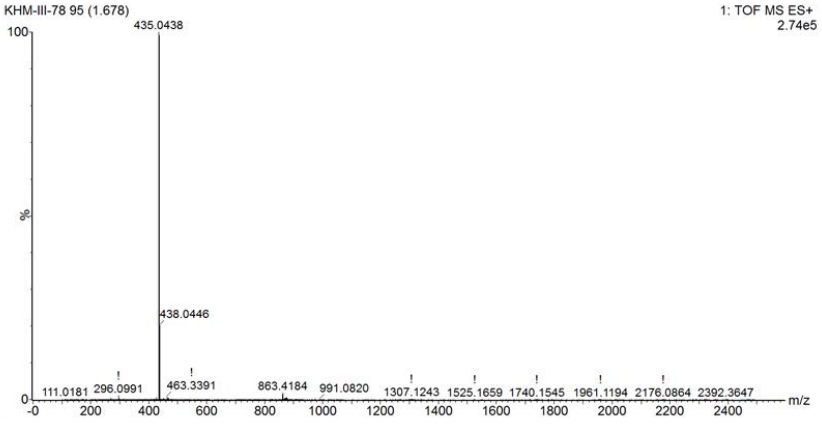
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

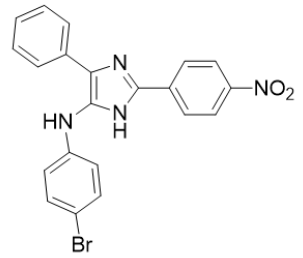
Monoisotopic Mass, Even Electron Ions
2083 formula(e) evaluated with 22 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

KHM-III-78 95 (1.678)
1: TOF MS ES+

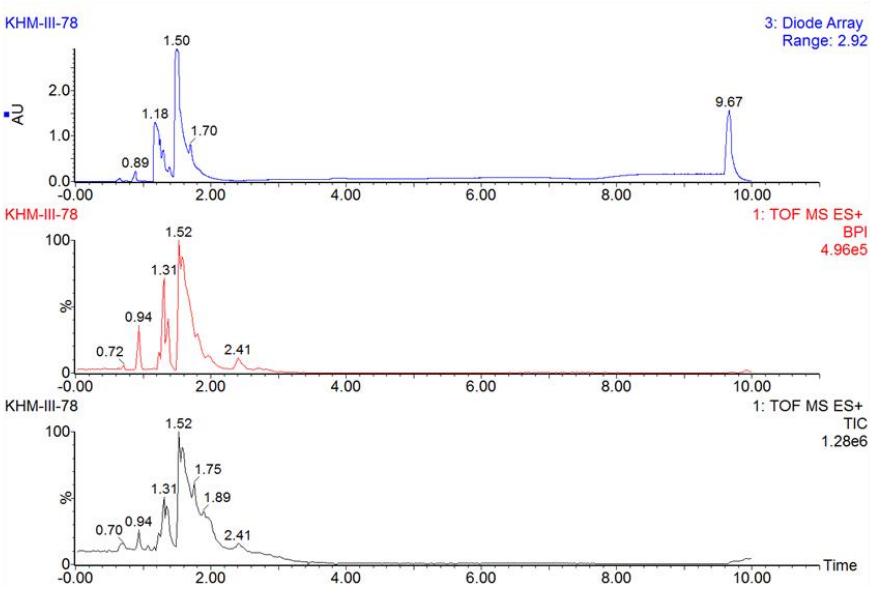


Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
435.0438	435.0443	-0.5	-1.1	10.5	330.3	0.628	53.38	C20 H20 O6 Br
	435.0416	2.2	5.1	11.5	330.6	0.909	40.29	C16 H16 N6 O4 Br
	435.0430	0.8	1.8	16.5	332.6	2.882	5.60	C17 H12 N10 Br
	435.0457	-1.9	-4.4	15.5	334.9	5.220	0.54	C21 H16 N4 O2 Br
	435.0403	3.5	8.0	6.5	336.0	6.312	0.18	C15 H20 N2 O8 Br
	435.0475	-3.7	-8.5	2.5	340.8	11.091	0.00	C9 H20 N6 O9 Br
	435.0435	0.3	0.7	-1.5	344.5	14.792	0.00	C4 H20 N8 O11 Br
	435.0395	4.3	9.9	4.5	344.8	15.109	0.00	C15 H25 N4 O Br2
	435.0467	-2.9	-6.7	0.5	345.3	15.599	0.00	C9 H25 N8 O2 Br2
	435.0470	-3.2	-7.4	-0.5	354.2	24.494	0.00	C8 H19 O20
	435.0411	2.7	6.2	8.5	354.3	24.625	0.00	C15 H15 O15
	435.0397	4.1	9.4	14.5	354.3	24.634	0.00	C12 H7 N10 O9
	435.0483	-4.5	-10.3	4.5	354.4	24.710	0.00	C9 H15 N4 O16
	435.0424	1.4	3.2	13.5	354.4	24.719	0.00	C16 H11 N4 O11
	435.0438	0.0	0.0	18.5	354.4	24.734	0.00	C17 H7 N8 O7
	435.0443	-0.5	-1.1	0.5	354.6	24.950	0.00	C4 H15 N6 O18
	435.0456	-1.8	-4.1	5.5	354.7	25.008	0.00	C5 H11 N10 O14
	435.0465	-2.7	-6.2	17.5	354.7	25.014	0.00	C21 H11 N2 O9
	435.0478	-4.0	-9.2	22.5	354.8	25.088	0.00	C22 H7 N6 O5
	435.0419	1.9	4.4	31.5	355.0	25.312	0.00	C29 H3 N6
	435.0406	3.2	7.4	26.5	355.0	25.316	0.00	C28 H7 N2 O4
	435.0446	-0.8	-1.8	30.5	355.3	25.574	0.00	C33 H7 O2





$[M+H]^+$: $C_{21}H_{16}N_4O_2Br$
Exact Mass: 435.0457



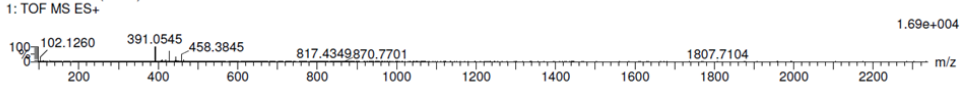
Compound 4ao

Elemental Composition Report

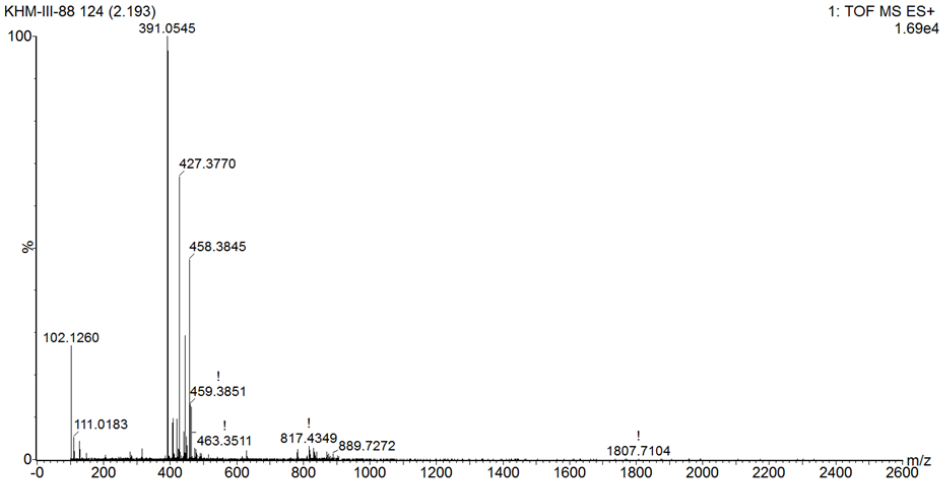
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

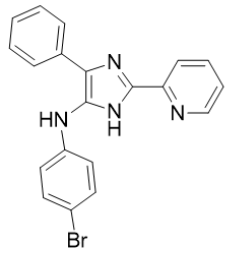
Monoisotopic Mass, Even Electron Ions
171 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

KHM-III-88 124 (2.193)
1: TOF MS ES+

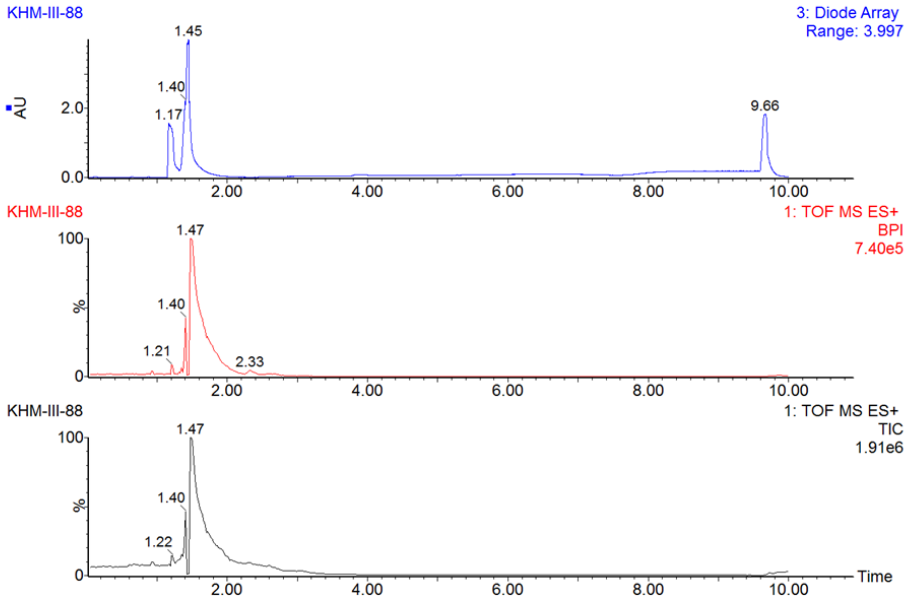


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
391.0545	391.0558	-1.3	-3.3	14.5	155.7	0.033	96.75	C20 H16 N4 Br
	391.0569	-2.4	-6.1	-0.5	159.1	3.428	3.25	C8 H25 N8 Br2
	391.0548	-0.3	-0.8	29.5	170.4	14.669	0.00	C32 H7





$[M+H]^+$: $C_{20}H_{16}N_4Br$
Exact Mass: 391.0558



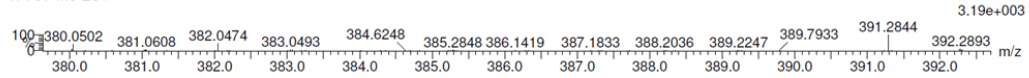
Compound 4ap

Elemental Composition Report

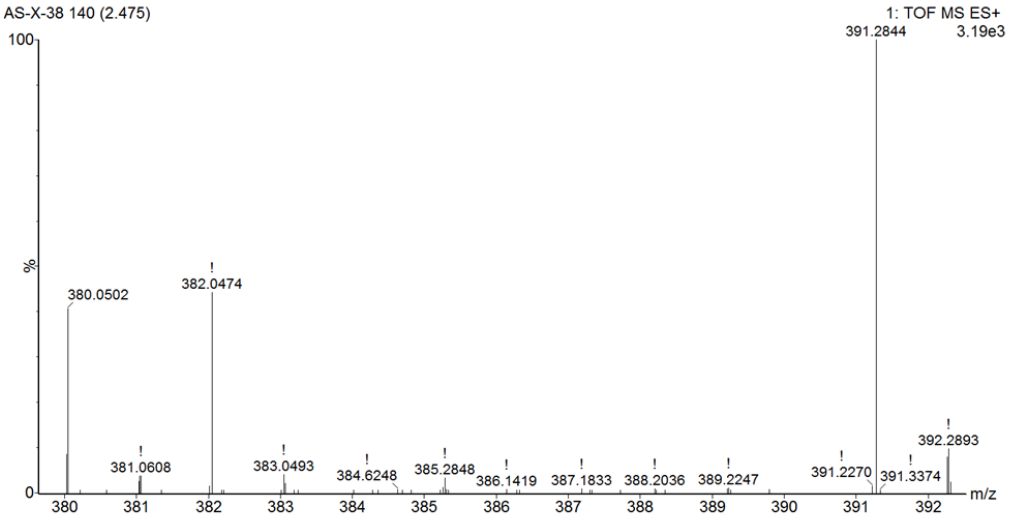
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

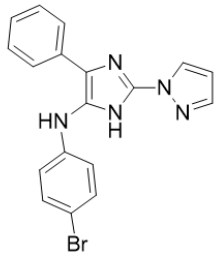
Monoisotopic Mass, Even Electron Ions
161 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

AS-X-38 140 (2.475)
1: TOF MS ES+

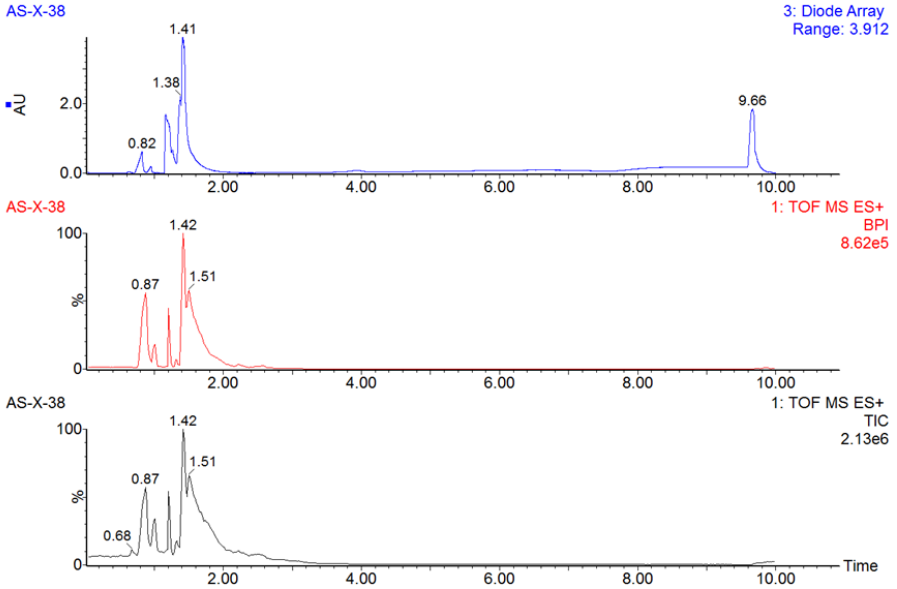


Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
380.0502	380.0521	-1.9	-5.0	-1.5	73.8	0.346	70.76	C6 H24 N9 Br2
	380.0511	-0.9	-2.4	13.5	74.7	1.230	29.23	C18 H15 N5 Br
	380.0500	0.2	0.5	28.5	83.0	9.531	0.01	C30 H6 N





$[M+H]^+$: $C_{18}H_{15}N_5Br$
Exact Mass: 380.0511



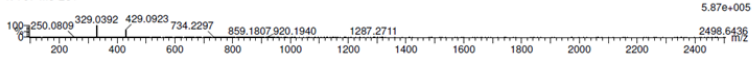
Compound 4aq

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

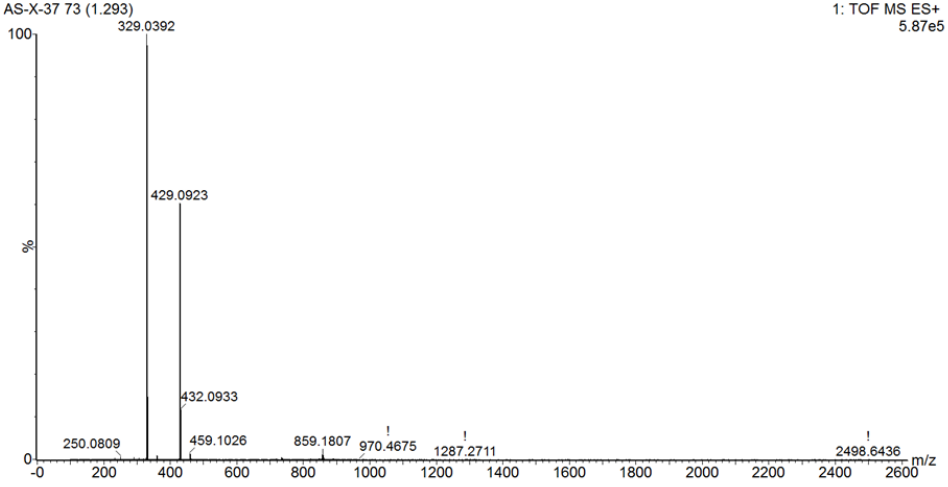
Monoisotopic Mass, Even Electron Ions
2025 formula(e) evaluated with 19 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

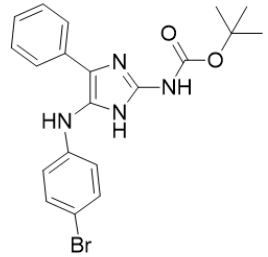
AS-X-37 73 (1.293)
1: TOF MS ES+
5.87e+005



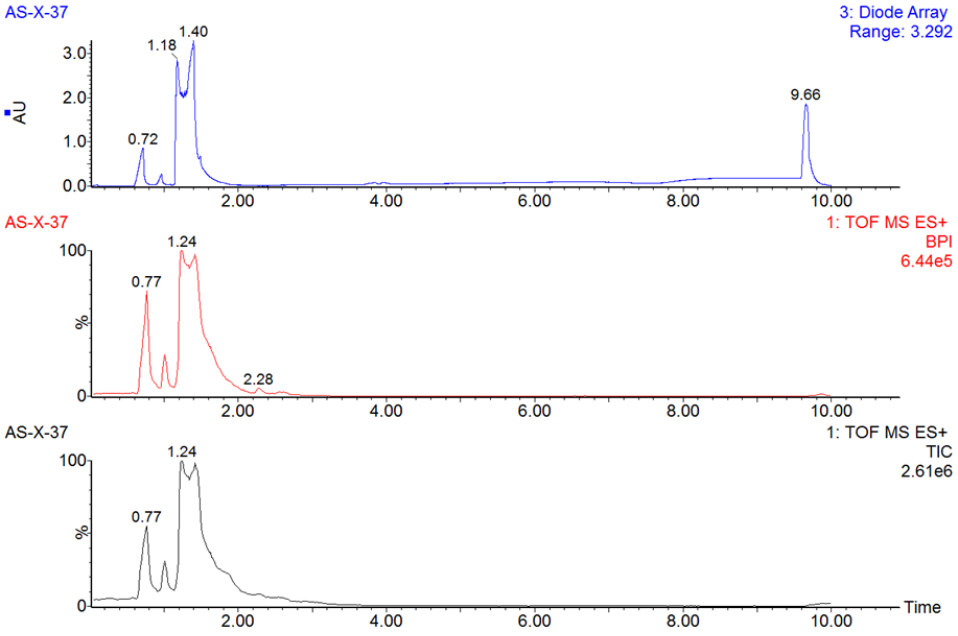
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
429.0923	429.0913	1.0	2.3	6.5	393.0	0.662	51.60	C19 H26 O6 Br
	429.0899	2.4	5.6	12.5	393.3	0.956	38.43	C16 H18 N10 Br
	429.0886	3.7	8.6	7.5	394.7	2.444	8.68	C15 H22 N6 O4 Br
	429.0926	-0.3	-0.7	11.5	396.7	4.370	1.26	C20 H22 N4 O2 Br
	429.0945	-2.2	-5.1	-1.5	401.2	8.849	0.01	C8 H26 N6 O9 Br
	429.0958	-3.5	-8.2	3.5	401.6	9.264	0.01	C9 H22 N10 O5 Br
	429.0966	-4.3	-10.0	15.5	402.9	10.600	0.00	C25 H22 N2 Br
	429.0880	4.3	10.0	4.5	416.5	24.151	0.00	C14 H21 O15
	429.0953	-3.0	-7.0	0.5	416.5	24.176	0.00	C8 H21 N4 O16
	429.0907	1.6	3.7	14.5	416.5	24.226	0.00	C16 H13 N8 O7
	429.0894	2.9	6.8	9.5	416.5	24.231	0.00	C15 H17 N4 O11
	429.0966	-4.3	-10.0	5.5	416.6	24.262	0.00	C9 H17 N8 O12
	429.0934	-1.1	-2.6	13.5	416.8	24.524	0.00	C20 H17 N2 O9
	429.0961	-3.8	-8.9	23.5	416.9	24.576	0.00	C22 H9 N10 O
	429.0947	-2.4	-5.6	18.5	416.9	24.579	0.00	C21 H13 N6 O5
	429.0926	-0.3	-0.7	1.5	416.9	24.590	0.00	C4 H17 N10 O14
	429.0889	3.4	7.9	27.5	417.2	24.886	0.00	C28 H9 N6
	429.0875	4.8	11.2	22.5	417.2	24.904	0.00	C27 H13 N2 O4
	429.0916	0.7	1.6	26.5	417.5	25.174	0.00	C32 H13 O2

AS-X-37 73 (1.293)
1: TOF MS ES+
5.87e5

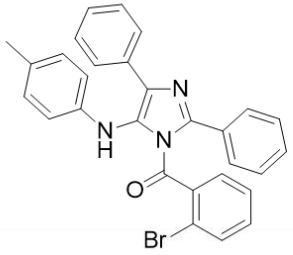




$[M+H]^+$: $C_{20}H_{22}BrN_4O_2$
Exact Mass: 429.0926



Compound 5a

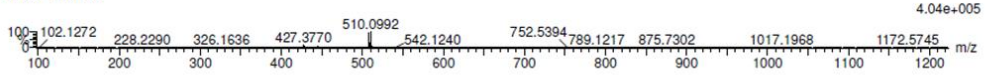


$[M+H]^+$: $C_{29}H_{23}BrN_3O$
Exact Mass: 508.1024

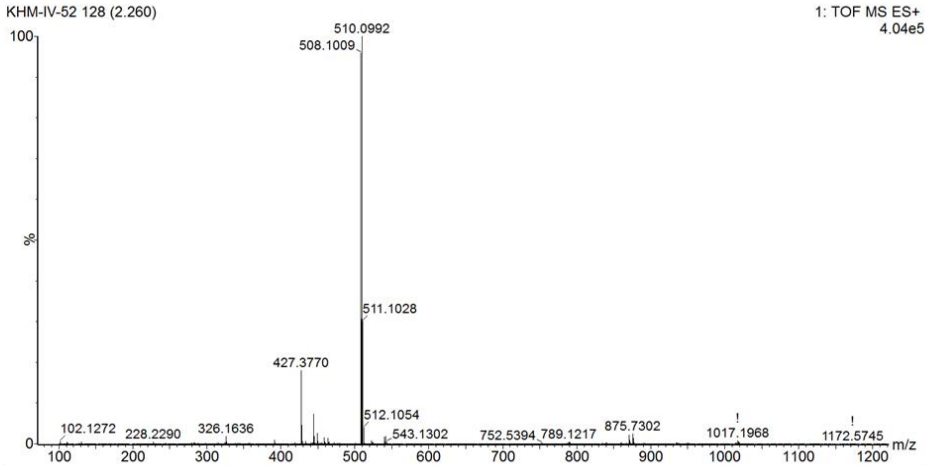
Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

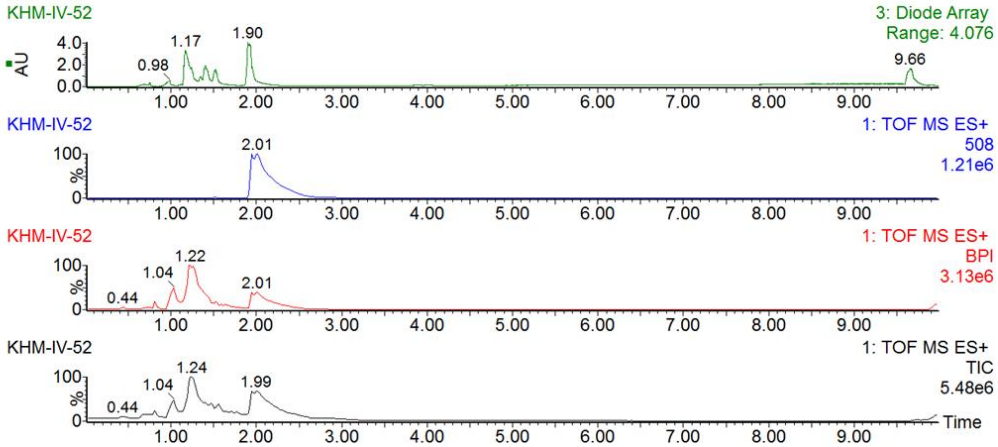
Monoisotopic Mass, Even Electron Ions
3036 formula(e) evaluated with 22 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

KHM-IV-52 128 (2.260)
1: TOF MS ES+
4.04e+005



Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
508.1009	508.1025	-1.6	-3.1	19.5	465.0	0.006	99.38	C29 H23 N3 O Br
	508.0984	2.5	4.9	15.5	470.1	5.177	0.56	C24 H23 N5 O3 Br
	508.0971	3.8	7.5	10.5	472.7	7.780	0.04	C23 H27 N O7 Br
	508.1030	-2.1	-4.1	1.5	474.4	9.427	0.01	C16 H31 N O12 Br
	508.1043	-3.4	-6.7	6.5	475.2	10.202	0.00	C17 H27 N5 O8 Br
	508.1056	-4.7	-9.3	11.5	475.5	10.503	0.00	C18 H23 N9 O4 Br
	508.1003	0.6	1.2	2.5	476.6	11.598	0.00	C12 H27 N7 O10 Br
	508.1022	-1.3	-2.6	-0.5	477.8	12.824	0.00	C16 H36 N3 O5 Br2
	508.1035	-2.6	-5.1	4.5	479.1	14.142	0.00	C17 H32 N7 O Br2
	508.0963	4.6	9.1	8.5	480.1	15.128	0.00	C23 H32 N3 Br2
	508.0995	1.4	2.8	0.5	480.3	15.352	0.00	C12 H32 N9 O3 Br2
	508.0963	4.6	9.1	-1.5	480.5	15.562	0.00	C7 H27 N9 O12 Br
	508.1011	-0.2	-0.4	4.5	488.8	23.857	0.00	C12 H22 N5 O17
	508.1024	-1.5	-3.0	9.5	488.8	23.885	0.00	C13 H18 N9 O13
	508.0965	4.4	8.7	18.5	488.9	23.922	0.00	C20 H14 N9 O8
	508.1051	-4.2	-8.3	8.5	489.0	24.019	0.00	C17 H22 N3 O15
	508.1006	0.3	0.6	22.5	489.0	24.047	0.00	C25 H14 N7 O6
	508.0992	1.7	3.3	17.5	489.0	24.057	0.00	C24 H18 N3 O10
	508.0970	3.9	7.7	0.5	489.0	24.083	0.00	C7 H22 N7 O19
	508.1032	-2.3	-4.5	21.5	489.2	24.284	0.00	C29 H18 N O8
	508.1046	-3.7	-7.3	26.5	489.3	24.305	0.00	C30 H14 N5 O4
	508.0974	3.5	6.9	30.5	489.4	24.395	0.00	C36 H14 N O3

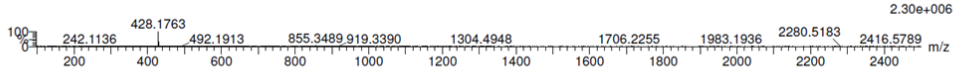




Compound 6a

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
843 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20
KHM-IV-53 117 (2.071)
1: TOF MS ES+



Minimum:				-1.5				
Maximum:		5.0	10.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
428.1763	428.1763	0.0	0.0	20.5	700.1	0.107	89.88	C29 H22 N3 O
	428.1723	4.0	9.3	16.5	702.3	2.311	9.92	C24 H22 N5 O3
	428.1795	-3.2	-7.5	12.5	707.1	7.048	0.09	C18 H22 N9 O4
	428.1781	-1.8	-4.2	7.5	707.1	7.063	0.09	C17 H26 N5 O8
	428.1768	-0.5	-1.2	2.5	708.4	8.362	0.02	C16 H30 N O12
	428.1741	2.2	5.1	3.5	710.3	10.242	0.00	C12 H26 N7 O10
	428.1728	3.5	8.2	-1.5	711.5	11.464	0.00	C11 H30 N3 O14